

index. Enter "HELP COMMANDS" at an arrow prompt (=>) for a list of commands which can be used in this file.

=> FILE REGISTRY

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	0.21	0.21

FILE 'REGISTRY' ENTERED AT 11:54:22 ON 22 JUN 2004  
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Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 21 JUN 2004 HIGHEST RN 697224-75-2  
DICTIONARY FILE UPDATES: 21 JUN 2004 HIGHEST RN 697224-75-2

TSCA INFORMATION NOW CURRENT THROUGH JANUARY 6, 2004

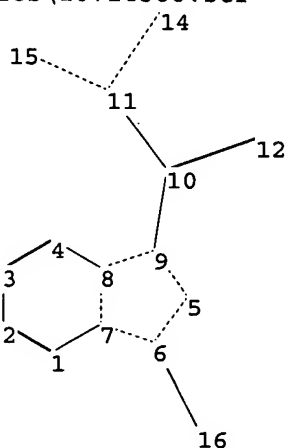
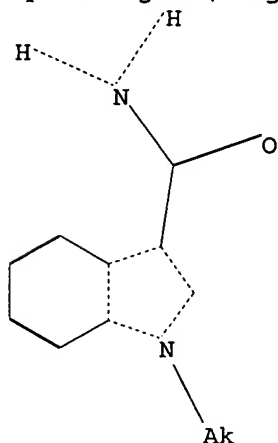
Please note that search-term pricing does apply when conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more information enter HELP PROP at an arrow prompt in the file or refer to the file summary sheet on the web at:  
<http://www.cas.org/ONLINE/DBSS/registryss.html>

=>

Uploading C:\Program Files\Stnexp\Queries\10714568.str



chain nodes :  
10 11 12 14 15 16  
ring nodes :  
1 2 3 4 5 6 7 8 9  
chain bonds :  
6-16 9-10 10-11 10-12 11-14 11-15  
ring bonds :  
1-2 1-7 2-3 3-4 4-8 5-6 5-9 6-7 7-8 8-9  
exact/norm bonds :

10714568

5-6 5-9 6-7 6-16 7-8 8-9 10-11 10-12 11-14 11-15

exact bonds :

1-2 1-7 2-3 3-4 4-8 9-10

isolated ring systems :

containing 1 :

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:CLASS

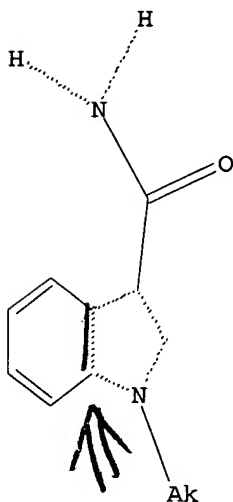
11:CLASS 12:CLASS 14:CLASS 15:CLASS 16:CLASS

L1 STRUCTURE UPLOADED

=&gt; d l1

L1 HAS NO ANSWERS

L1 STR



Structure attributes must be viewed using STN Express query preparation.

=&gt; s l1

SAMPLE SEARCH INITIATED 11:54:39 FILE 'REGISTRY'

SAMPLE SCREEN SEARCH COMPLETED - 102 TO ITERATE

100.0% PROCESSED 102 ITERATIONS

0 ANSWERS

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*

BATCH \*\*COMPLETE\*\*

PROJECTED ITERATIONS: 1435 TO 2645

PROJECTED ANSWERS: 0 TO 0

L2 0 SEA SSS SAM L1

=&gt; s l1 sss full

FULL SEARCH INITIATED 11:54:45 FILE 'REGISTRY'

FULL SCREEN SEARCH COMPLETED - 2436 TO ITERATE

10714568

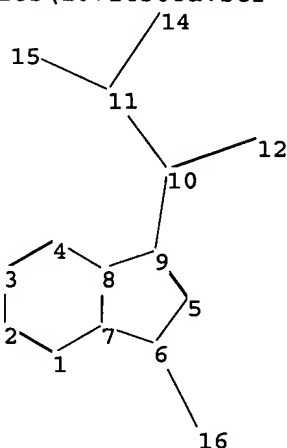
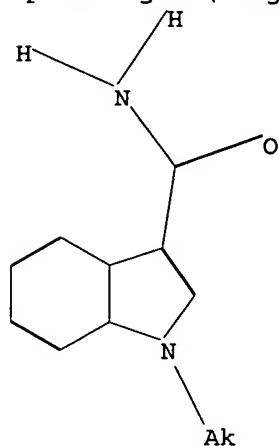
100.0% PROCESSED 2436 ITERATIONS  
SEARCH TIME: 00.00.01

0 ANSWERS

L3 0 SEA SSS FUL L1

=>

Uploading C:\Program Files\Stnexp\Queries\10714568a.str



chain nodes :

10 11 12 14 15 16

ring nodes :

1 2 3 4 5 6 7 8 9

chain bonds :

6-16 9-10 10-11 10-12 11-14 11-15

ring bonds :

1-2 1-7 2-3 3-4 4-8 5-6 5-9 6-7 7-8 8-9

exact/norm bonds :

5-6 6-7 6-16 10-11 10-12

exact bonds :

1-2 1-7 2-3 3-4 4-8 5-9 7-8 8-9 9-10 11-14 11-15

isolated ring systems :

containing 1 :

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:CLASS  
11:CLASS 12:CLASS 14:CLASS 15:CLASS 16:CLASS

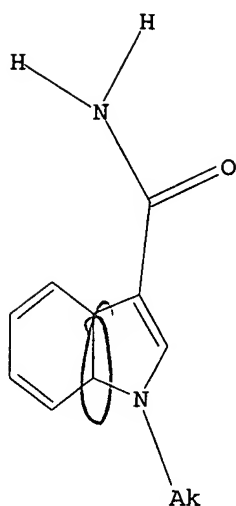
L4 STRUCTURE UPLOADED

=> d 14

L4 HAS NO ANSWERS

L4 STR

10714568



Structure attributes must be viewed using STN Express query preparation.

=> s l4

SAMPLE SEARCH INITIATED 11:56:27 FILE 'REGISTRY'  
SAMPLE SCREEN SEARCH COMPLETED - 9 TO ITERATE

100.0% PROCESSED 9 ITERATIONS  
SEARCH TIME: 00.00.01

~~0 ANSWERS~~

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*  
BATCH \*\*COMPLETE\*\*  
PROJECTED ITERATIONS: 9 TO 360  
PROJECTED ANSWERS: 0 TO 0

L5 0 SEA SSS SAM L4

=> s l4 sss full

FULL SEARCH INITIATED 11:56:34 FILE 'REGISTRY'  
FULL SCREEN SEARCH COMPLETED - 210 TO ITERATE

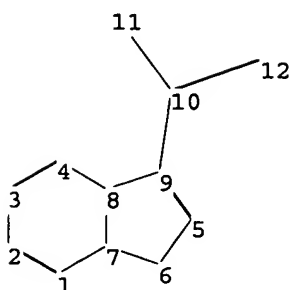
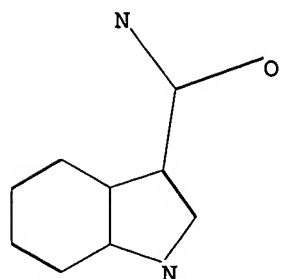
100.0% PROCESSED 210 ITERATIONS  
SEARCH TIME: 00.00.01

✓  
0 ANSWERS

L6 0 SEA SSS FUL L4

=>

Uploading C:\Program Files\Stnexp\Queries\10714568c.str



```

chain nodes :
10 11 12
ring nodes :
1 2 3 4 5 6 7 8 9
chain bonds :
9-10 10-11 10-12
ring bonds :
1-2 1-7 2-3 3-4 4-8 5-6 5-9 6-7 7-8 8-9
exact/norm bonds :
5-6 6-7 10-11 10-12
exact bonds :
1-2 1-7 2-3 3-4 4-8 5-9 7-8 8-9 9-10
isolated ring systems :
containing 1 :
```

Match level :

```

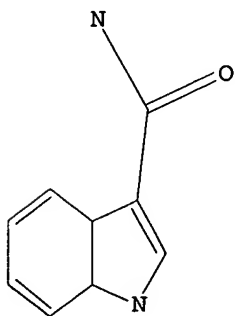
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:CLASS
11:CLASS 12:CLASS
```

L7 STRUCTURE UPLOADED

=> d 17

L7 HAS NO ANSWERS

L7 STR



Structure attributes must be viewed using STN Express query preparation.

=> s 17

10714568

SAMPLE SEARCH INITIATED 11:57:56 FILE 'REGISTRY'  
 SAMPLE SCREEN SEARCH COMPLETED - 9 TO ITERATE

100.0% PROCESSED 9 ITERATIONS  
 SEARCH TIME: 00.00.01

0 ANSWERS

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*  
 BATCH \*\*COMPLETE\*\*  
 PROJECTED ITERATIONS: 9 TO 360  
 PROJECTED ANSWERS: 0 TO 0

L8 0 SEA SSS SAM L7

=> s l7 sss full

FULL SEARCH INITIATED 11:58:03 FILE 'REGISTRY'  
 FULL SCREEN SEARCH COMPLETED - 210 TO ITERATE

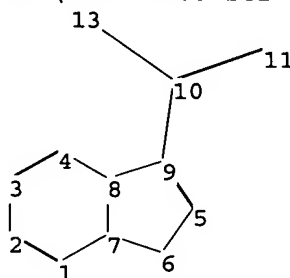
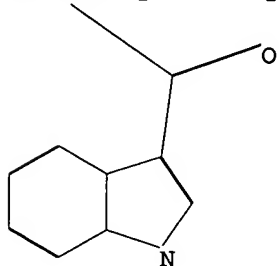
100.0% PROCESSED 210 ITERATIONS  
 SEARCH TIME: 00.00.01

0 ANSWERS

L9 0 SEA SSS FUL L7

=>

Uploading C:\Program Files\Stnexp\Queries\10714568d.str



chain nodes :

10 11 13

ring nodes :

1 2 3 4 5 6 7 8 9

chain bonds :

9-10 10-11 10-13

ring bonds :

1-2 1-7 2-3 3-4 4-8 5-6 5-9 6-7 7-8 8-9

exact/norm bonds :

5-6 6-7 10-11

exact bonds :

1-2 1-7 2-3 3-4 4-8 5-9 7-8 8-9 9-10 10-13

isolated ring systems :

containing 1 :

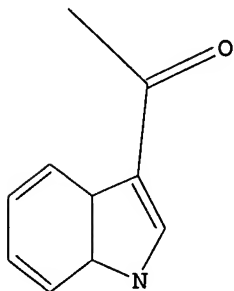
Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:CLASS  
 11:CLASS 13:CLASS

L10 STRUCTURE UPLOADED

10714568

=> d l10  
L10 HAS NO ANSWERS  
L10 STR



Structure attributes must be viewed using STN Express query preparation.

=> s l10  
SAMPLE SEARCH INITIATED 12:01:35 FILE 'REGISTRY'  
SAMPLE SCREEN SEARCH COMPLETED - 11 TO ITERATE

100.0% PROCESSED 11 ITERATIONS 1 ANSWERS  
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*  
BATCH \*\*COMPLETE\*\*  
PROJECTED ITERATIONS: 22 TO 418  
PROJECTED ANSWERS: 1 TO 80

L11 1 SEA SSS SAM L10

=> s l10 sss full  
FULL SEARCH INITIATED 12:01:42 FILE 'REGISTRY'  
FULL SCREEN SEARCH COMPLETED - 257 TO ITERATE

100.0% PROCESSED 257 ITERATIONS  
SEARCH TIME: 00.00.01

L12 1 SEA SSS FUL L10

=> FIL CAPLUS  
COST IN U.S. DOLLARS  
FULL ESTIMATED COST

SINCE FILE	TOTAL
ENTRY	SESSION
625.04	625.25

FILE 'CAPLUS' ENTERED AT 12:01:50 ON 22 JUN 2004  
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FILE COVERS 1907 - 22 Jun 2004 VOL 140 ISS 26  
FILE LAST UPDATED: 21 Jun 2004 (20040621/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s l12

L13 0 L12

=> d his

(FILE 'HOME' ENTERED AT 11:53:52 ON 22 JUN 2004)

FILE 'REGISTRY' ENTERED AT 11:54:22 ON 22 JUN 2004

L1 STRUCTURE UPLOADED  
L2 0 S L1  
L3 0 S L1 SSS FULL  
L4 STRUCTURE UPLOADED  
L5 0 S L4  
L6 0 S L4 SSS FULL  
L7 STRUCTURE UPLOADED  
L8 0 S L7  
L9 0 S L7 SSS FULL  
L10 STRUCTURE UPLOADED  
L11 1 S L10  
L12 1 S L10 SSS FULL

FILE 'CAPLUS' ENTERED AT 12:01:50 ON 22 JUN 2004

L13 0 S L12

=> s l12

L14 0 L12

=> FIL REGISTRY

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

3.07

628.32

FILE 'REGISTRY' ENTERED AT 12:06:06 ON 22 JUN 2004

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STRUCTURE FILE UPDATES: 21 JUN 2004 HIGHEST RN 697224-75-2

DICTIONARY FILE UPDATES: 21 JUN 2004 HIGHEST RN 697224-75-2

TSCA INFORMATION NOW CURRENT THROUGH JANUARY 6, 2004

Please note that search-term pricing does apply when conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

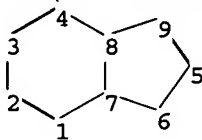
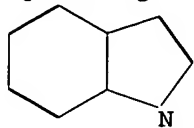
10714568



Experimental and calculated property data are now available. For more information enter HELP PROP at an arrow prompt in the file or refer to the file summary sheet on the web at:  
<http://www.cas.org/ONLINE/DBSS/registryss.html>

=&gt;

Uploading C:\Program Files\Stnexp\Queries\10714568e.str



ring nodes :

1 2 3 4 5 6 7 8 9

ring bonds :

1-2 1-7 2-3 3-4 4-8 5-6 5-9 6-7 7-8 8-9

exact/norm bonds :

5-6 6-7

exact bonds :

1-2 1-7 2-3 3-4 4-8 5-9 7-8 8-9

isolated ring systems :

containing 1 :

Match level :

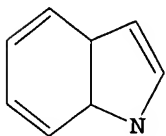
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom

L15 STRUCTURE UPLOADED

=> d l15

L15 HAS NO ANSWERS

L15 STR



Structure attributes must be viewed using STN Express query preparation.

=> s l15

SAMPLE SEARCH INITIATED 12:06:26 FILE 'REGISTRY'

SAMPLE SCREEN SEARCH COMPLETED - 2869 TO ITERATE

34.9% PROCESSED 1000 ITERATIONS  
 INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)  
 SEARCH TIME: 00.00.01

2 ANSWERS

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*

BATCH \*\*COMPLETE\*\*

PROJECTED ITERATIONS: 54168 TO 60592

10714568

PROJECTED ANSWERS: 2 TO 257

L16 2 SEA SSS SAM L15

=> s l15 sss full  
FULL SEARCH INITIATED 12:06:33 FILE 'REGISTRY'  
FULL SCREEN SEARCH COMPLETED - 56102 TO ITERATE

100.0% PROCESSED 56102 ITERATIONS 89 ANSWERS  
SEARCH TIME: 00.00.01

L17 89 SEA SSS FUL L15

=> FIL CAPLUS  
COST IN U.S. DOLLARS SINCE FILE TOTAL  
ENTRY SESSION  
FULL ESTIMATED COST 155.42 783.74

FILE 'CAPLUS' ENTERED AT 12:06:39 ON 22 JUN 2004  
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FILE COVERS 1907 - 22 Jun 2004 VOL 140 ISS 26  
FILE LAST UPDATED: 21 Jun 2004 (20040621/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s l17  
L18 34 L17  
=> s l18 and py<=2002  
22503583 PY<=2002  
L19 29 L18 AND PY<=2002

=> s l19 and thu  
138 THU  
2162536 THUS  
2162659 THU  
(THU OR THUS)  
L20 9 L19 AND THU

=> d l20 ibib abs hitstr tot

L20 ANSWER 1 OF 9 CAPLUS COPYRIGHT 2004 ACS on STN  
ACCESSION NUMBER: 2000:181089 CAPLUS  
DOCUMENT NUMBER: 132:209146

10714568

TITLE: Lightfast coloring agents and image recording materials, thermal transfer materials, and ink-jet recording fluids containing them

INVENTOR(S): Oya, Hidenobu; Kaneko, Manabu; Kida, Shuji

PATENT ASSIGNEE(S): Konica Co., Japan

SOURCE: Jpn. Kokai Tokkyo Koho, 46 pp.  
CODEN: JKXXAF

DOCUMENT TYPE: Patent

LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 2

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 2000080295	A2	20000321	JP 1999-143284	19990524 <--
PRIORITY APPLN. INFO.:			JP 1998-193794	A 19980624

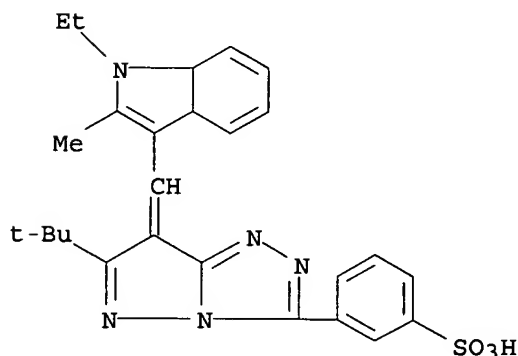
OTHER SOURCE(S): MARPAT 132:209146

AB The coloring agents represented by AN:B [I; B = coupler component binding to N at an active site; A = N-containing heterocyclic or heteropolycyclic ring, where  $\geq 1$  N in the ring is placed at an end of conjugation to form conjugated chain with N:B; except A being amino-substituted hetero ring and B being (un)substituted phenol] are prepared. Other coloring agents AC(R1):B (R1 = H, substituent), etc., are also claimed. Thus, a MEK-based thermal transfer ink containing I [A = 1-tert-butyl-3-pyrrolyl; B = C(OCMe<sub>3</sub>)CONH-o-C<sub>6</sub>H<sub>4</sub>OMe] and polyvinyl butyral (BL 1) formed a light-resistant yellow image. Syntheses of several colorants were exemplified.

IT 260801-71-6 260801-72-7  
RL: PRP (Properties); TEM (Technical or engineered material use); USES (Uses)  
(lightfast coloring agents for image recording materials, thermal transfer materials, and ink-jet recording fluids)

RN 260801-71-6 CAPLUS

CN Benzenesulfonic acid, 3-[6-(1,1-dimethylethyl)-7-[(1-ethyl-3a,7a-dihydro-2-methyl-1H-indol-3-yl)methylene]-7H-pyrazolo[5,1-c]-1,2,4-triazol-3-yl]-, sodium salt (9CI) (CA INDEX NAME)

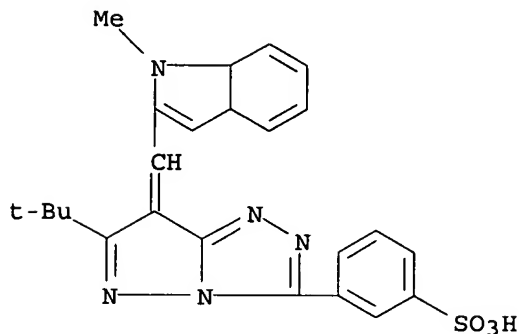


● Na

RN 260801-72-7 CAPLUS

CN Benzenesulfonic acid, 3-[7-[(3a,7a-dihydro-1-methyl-1H-indol-2-yl)methylene]-6-(1,1-dimethylethyl)-7H-pyrazolo[5,1-c]-1,2,4-triazol-3-yl]-

, sodium salt (9CI) (CA INDEX NAME)



● Na

L20 ANSWER 2 OF 9 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1999:325961 CAPLUS

DOCUMENT NUMBER: 130:352553

TITLE: Synthesis of dipeptide nitriles as inhibitors of cysteine cathepsins

INVENTOR(S): Altmann, Eva; Betschart, Claudia; Gohda, Keigo; Horiuchi, Miyuki; Lattmann, Rene; Missbach, Martin; Sakaki, Junichi; Takai, Michihiro; Teno, Naoki; Cowen, Scott Douglas; Greenspan, Paul David; McQuire, Leslie Wighton; Tommasi, Ruben Alberto; Van Duzer, John Henry

PATENT ASSIGNEE(S): Novartis AG, Switz.; Novartis-Erfindungen Verwaltungsgesellschaft mbH

SOURCE: PCT Int. Appl., 137 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9924460	A2	19990520	WO 1998-EP6937	19981103 <--
WO 9924460	A3	19990902		
W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
CA 2306313	AA	19990520	CA 1998-2306313	19981103 <--
AU 9914873	A1	19990531	AU 1999-14873	19981103 <--
AU 751669	B2	20020822		
EP 1028942	A2	20000823	EP 1998-958887	19981103 <--
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI				
BR 9813197	A	20000829	BR 1998-13197	19981103 <--

TR 200001189	T2	20000921	TR 2000-200001189	19981103	<--
JP 2001522862	T2	20011120	JP 2000-520468	19981103	<--
RU 2201420	C2	20030327	RU 2000-114821	19981103	
ZA 9810073	A	19990505	ZA 1998-10073	19981104	<--
TW 527362	B	20030411	TW 1998-87118553	19981105	
NO 2000002320	A	20000704	NO 2000-2320	20000502	<--
US 6353017	B1	20020305	US 2000-643639	20000822	<--
US 2004029814	A1	20040212	US 2003-342872	20030115	
US 2004110806	A1	20040610	US 2003-694672	20031028	

PRIORITY APPLN. INFO.:

GB 1997-23407	A	19971105
US 1997-108160P	P	19971205
US 1997-985973	A	19971205
WO 1998-EP6937	W	19981103
US 1998-186223	B1	19981104
US 2000-643639	A1	20000822
US 2002-54590	B1	20020122
US 2003-342872	A1	20030115

OTHER SOURCE(S): MARPAT 130:352553

AB N-terminal substituted dipeptide nitriles R(L)xX1NHCR2R3C(:Y)NHCR4R5CN [R is optionally substituted aryl, alkyl, alkenyl, alkynyl, heterocyclyl; R2, R3 = H, optionally substituted alkyl, cycloalkyl, bicycloalkyl, or aryl-, biaryl-, cycloalkyl, bicycloalkylalkyl; R2 and R3 together represent alkylene, optionally interrupted by O, S, or NR6, where R6 is H, alkyl, arylalkyl; or R2 or R3 are linked by alkylene to the adjacent nitrogen to form a ring; R4, R5 = H, optionally substituted alkyl, arylalkyl, CO2R7, CONR7R8 (R7 is optionally substituted alkyl, aryl, arylalkyl, cycloalkyl, bicycloalkyl, or heterocyclyl and R8 is H or optionally substituted alkyl, aryl, arylalkyl, cycloalkyl, bicycloalkyl, heterocyclyl), etc.; R4 and R5 together represent alkylene, optionally interrupted by O, S, or NR6; X1 = CO, CS, SO, SO2, P(O)OR6; Y = O, S: L is optionally substituted Het, Het-CH2, CH2-Het (Het = O, N, or S); x = zero or 1] were prepared as inhibitors of cysteine cathepsins, e.g., cathepsins B, K, L and S, and can be used for the treatment of cysteine cathepsin dependent diseases and conditions. Thus, N-[2-[(3-carboxyphenyl)methoxy]-1(S)-cyanoethyl]-3-methyl-N $\alpha$ -(2,2-diphenylacetyl)-L-phenylalaninamide was prepared and shown to have IC50  $\approx$  5 nM for inhibition of cathepsin B.

IT 225119-82-4P

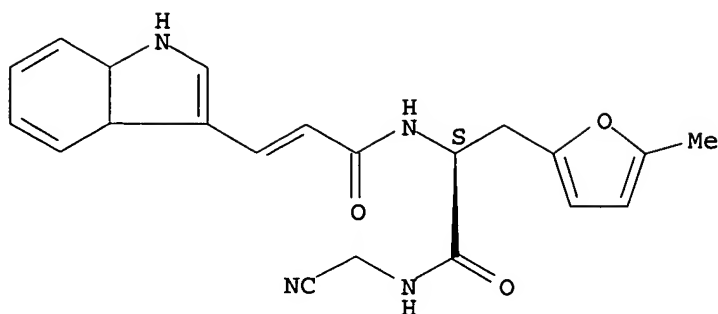
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)  
(synthesis of dipeptide nitriles as inhibitors of cysteine cathepsins)

RN 225119-82-4 CAPLUS

CN 2-Furanpropanamide, N-(cyanomethyl)- $\alpha$ -[[3-(3a,7a-dihydro-1H-indol-3-yl)-1-oxo-2-propenyl]amino]-5-methyl-, ( $\alpha$ S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry unknown.



L20 ANSWER 3 OF 9 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1998:1473 CAPLUS

DOCUMENT NUMBER: 128:61805

TITLE: Preparation of pyridylsulfonyl amino acid amide derivatives as thrombin inhibitors

INVENTOR(S): Brundish, Derek Edward; Brown, Lyndon Nigel; Le Grand, Darren Mark; Menear, Keith Allan; Smith, Garrick Paul; Allen, Mark Christopher; Butler, Paul Ian; Cockcroft, Xiao-Ling; Matthews, Ian Timothy William; Walker, Clive Victor; et al.

PATENT ASSIGNEE(S): Novartis A.-G., Switz.

SOURCE: PCT Int. Appl., 111 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9746553	A1	19971211	WO 1997-GB1385	19970521 <--
W: AL, AU, BA, BB, BG, BR, CA, CN, CU, CZ, EE, GE, GH, HU, IL, IS, JP, KP, KR, LC, LK, LR, LT, LV, MG, MK, MN, MX, NO, NZ, PL, RO, SG, SI, SK, TR, TT, UA, US, UZ, VN, YU, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, KE, LS, MW, SD, SZ, UG, AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
AU 9729081	A1	19980105	AU 1997-29081	19970521 <--
ZA 9704779	A	19971201	ZA 1997-4779	19970530 <--
PRIORITY APPLN. INFO.:			GB 1996-11461	A 19960601
			WO 1997-GB1385	W 19970521
OTHER SOURCE(S):			MARPAT 128:61805	
GI				

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

AB The present invention provides pyridylsulfonylamino acid amides I {Y = primary or secondary amino, group Q; A and R are absent; A = CH<sub>2</sub>, CH<sub>2</sub>CH<sub>2</sub>, R = H, halo, N<sub>3</sub>, CO<sub>2</sub>R<sub>8</sub>, SR<sub>12</sub>; B = CH or absent, provided that when B is absent, A and R are also absent; R<sub>1</sub> = H, alkyl, optionally substituted alkyl optionally interrupted by O, S, carboxylaminocarbonyl,

carbonylamino; optionally substituted Ph ring, Ph ring containing 1 or more heteroatoms, cyclohexane or bicyclic ring containing 1 or more heteroatoms; R2 = natural or synthetic amino acid residue; R3 = H, C1-8 alkyl optionally substituted by OH or halo; X = (CH2)n, CH2N, fused Ph ring optionally substituted by 1 or 2 methoxy groups; R8 = H, alkyl, OR9; R9 = H, alkyl, (un)substituted hydroxyalkyl, (un)substituted carboxyalkyl, (un)substituted amidoalkyl, SO2-alkyl, SO2-aryl, NR10R11; R10, R11 = independently H, optionally substituted alkyl optionally interrupted by O, MeSO2; NR10R11 = ring optionally containing another heteroatom; R12 = H, hydroxyalkyl; m = 0-2; n = 1-3] or a salt thereof. **Thus,** sulfonylation of benzothiazolylamino acid amide II (preparation given) with 4-chloro-3-pyridinesulfonyl chloride, followed by pyridine substitution with (S)-2-amino-3-phenyl-1-propanol gave desired thrombin inhibitor III. III inhibited human  $\alpha$ -thrombin with  $K_i$  = 6 nM.

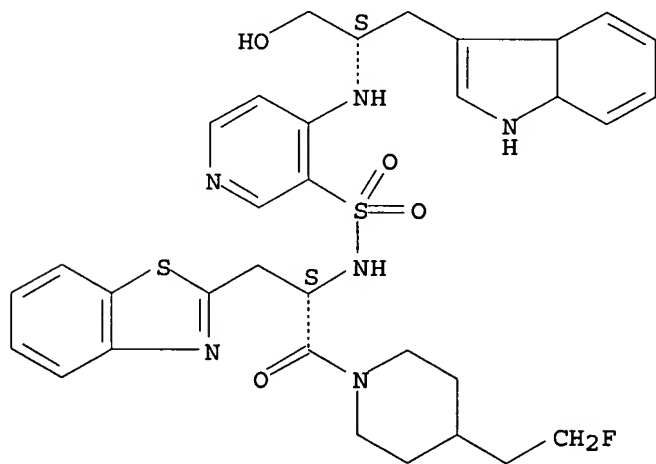
IT 200268-41-3P 200268-42-4P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)  
(preparation of pyridylsulfonyl amino acid amide derivs. as thrombin inhibitors)

RN 200268-41-3 CAPLUS

CN Piperidine, 1-[3-(2-benzothiazolyl)-2-[[[4-[[2-(3a,7a-dihydro-1H-indol-3-yl)-1-(hydroxymethyl)ethyl]amino]-3-pyridinyl]sulfonyl]amino]-1-oxopropyl]-4-(2-fluoroethyl)-, [3[S(S)]]-[partial]- (9CI) (CA INDEX NAME)

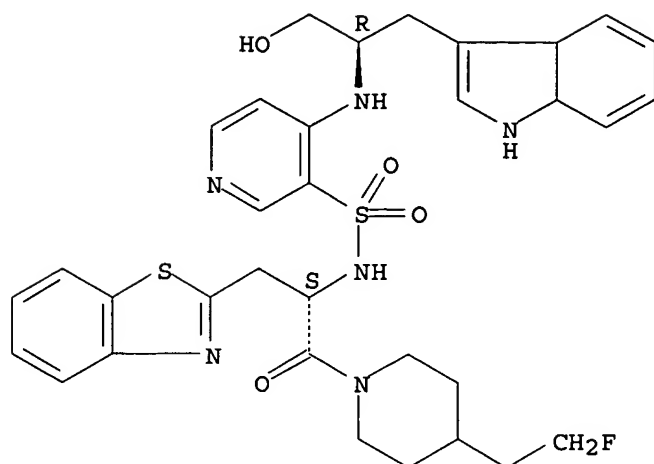
Absolute stereochemistry.



RN 200268-42-4 CAPLUS

CN Piperidine, 1-[3-(2-benzothiazolyl)-2-[[[4-[[2-(3a,7a-dihydro-1H-indol-3-yl)-1-(hydroxymethyl)ethyl]amino]-3-pyridinyl]sulfonyl]amino]-1-oxopropyl]-4-(2-fluoroethyl)-, [3[R(S)]]-[partial]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L20 ANSWER 4 OF 9 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1997:240627 CAPLUS

DOCUMENT NUMBER: 126:225294

TITLE: Preparation of pyrrolidine derivatives as phospholipase A2 inhibitors

INVENTOR(S): Ohtani, Mitsuaki; Kato, Toshiyuki; Watanabe, Fumihiko; Seno, Kaoru

PATENT ASSIGNEE(S): Shionogi and Co., Ltd., Japan

SOURCE: PCT Int. Appl., 129 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9705135	A1	19970213	WO 1996-JP2079	19960725 <--
W: AL, AM, AT, AU, AZ, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, HU, IL, IS, JP, KE, KG, KR, KZ, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG				
RW: KE, LS, MW, SD, SZ, UG, AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA				
CA 2227829	AA	19970213	CA 1996-2227829	19960725 <--
AU 9665308	A1	19970226	AU 1996-65308	19960725 <--
AU 707537	B2	19990715		
EP 848004	A1	19980617	EP 1996-925076	19960725 <--
EP 848004	B1	20030402		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI				
CN 1197458	A	19981028	CN 1996-197208	19960725 <--
CN 1064682	B	20010418		
BR 9609744	A	19990302	BR 1996-9744	19960725 <--
AT 236154	E	20030415	AT 1996-925076	19960725
PT 848004	T	20030731	PT 1996-925076	19960725
ES 2196163	T3	20031216	ES 1996-925076	19960725
US 5955616	A	19990921	US 1998-11404	19980128 <--
HK 1016598	A1	20010824	HK 1999-101691	19990420 <--



PRIORITY APPLN. INFO.:

JP 1995-194648

A 19950731

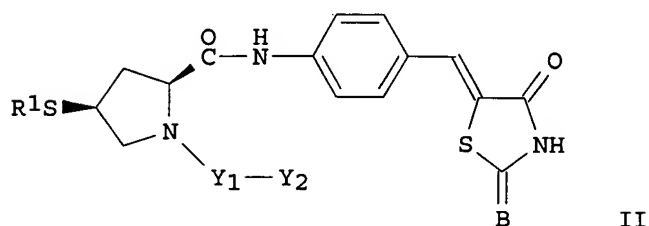
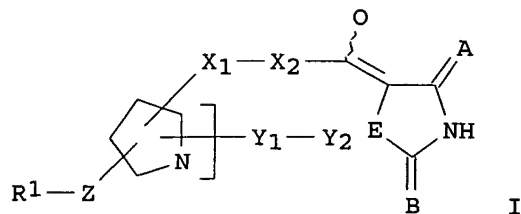
WO 1996-JP2079

W 19960725

OTHER SOURCE(S):

MARPAT 126:225294

GI



AB The title compds. [I; R1 = H, (un)substituted alkyl, alkenyl, or aralkyl, etc.; A, B, E = O, S; X1 = CO, CONH, CH2NHSO2, etc.; X2 = (un)substituted arylene or indole-1-yl, single bond; D = H, hydroxyalkyl; Y1 = (CH2)mCO, (CH2)nNHCO, etc.; m, n = 0-3; Y2 = H, alkyl, (un)substituted alkenyl, etc.; Z = S, SO, O, NH, CONH, CONHCH2, single bond] and pharmaceutically acceptable salts thereof are prepared I have the activity of inhibiting the production of prostaglandin E2 by inhibiting intracellular phospholipase A2. I, having the activity of inhibiting the production of prostaglandin E2 by inhibiting intracellular phospholipase A2, are useful for prevention and treatment of rheumatoid arthritis, asthma, allergic rhinitis, and related diseases. Thus, the title compound (II; R1 = C6H4CH2, Y2-Y1 = C6H4CO, B = S), which was prepared by 13 step reactions, showed IC50 of 7.2  $\mu$ M cPLA2 inhibitory activity.

IT 188109-01-5P 188109-02-6P 188109-03-7P

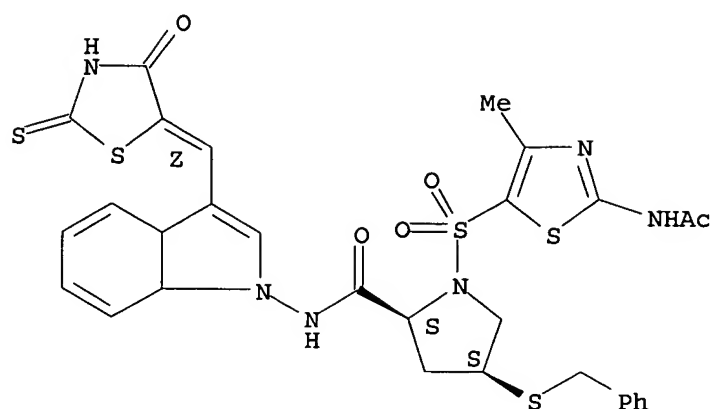
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)  
(preparation of pyrrolidine derivs. as phospholipase A2 inhibitors)

RN 188109-01-5 CAPLUS

CN 2-Pyrrolidinecarboxamide, 1-[[2-(acetylamino)-4-methyl-5-thiazolyl]sulfonyl]-N-[3a,7a-dihydro-3-[(4-oxo-2-thioxo-5-thiazolidinylidene)methyl]-1H-indol-1-yl]-4-[(phenylmethyl)thio]-, [1(2S,4S),3(Z)]-[partial]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

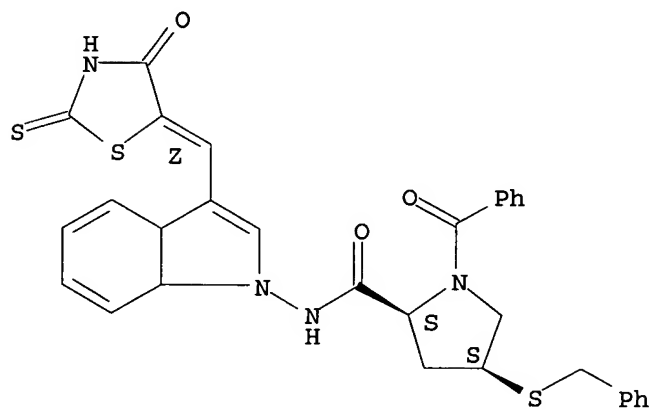
Double bond geometry as shown.



RN 188109-02-6 CAPLUS

CN 2-Pyrrolidinecarboxamide, 1-benzoyl-N-[3a,7a-dihydro-3-[(4-oxo-2-thioxo-5-thiazolidinylidene)methyl]-1H-indol-1-yl]-4-[(phenylmethyl)thio]-, [1(2S,4S),3(Z)]-[partial]- (9CI) (CA INDEX NAME)

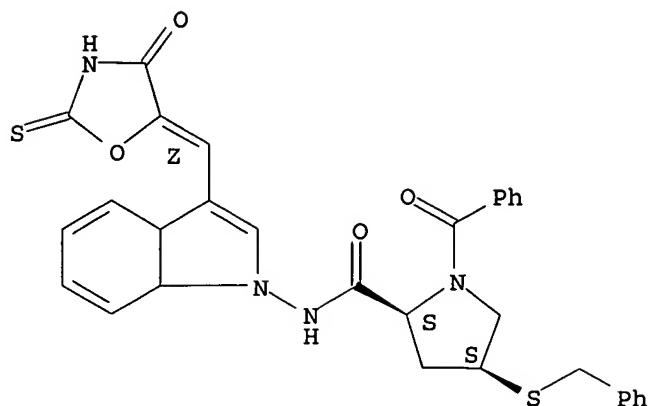
Absolute stereochemistry.  
Double bond geometry as shown.



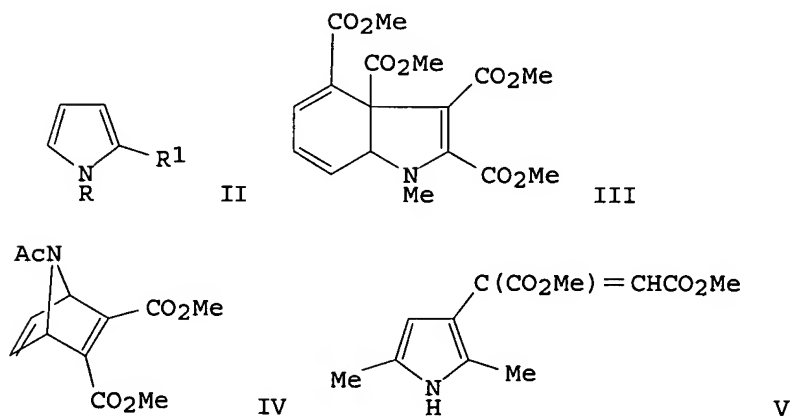
RN 188109-03-7 CAPLUS

CN 2-Pyrrolidinecarboxamide, 1-benzoyl-N-[3a,7a-dihydro-3-[(4-oxo-2-thioxo-5-oxazolidinylidene)methyl]-1H-indol-1-yl]-4-[(phenylmethyl)thio]-, [1(2S,4S),3(Z)]-[partial]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.  
Double bond geometry as shown.



L20 ANSWER 5 OF 9 CAPLUS COPYRIGHT 2004 ACS on STN  
 ACCESSION NUMBER: 1983:53585 CAPLUS  
 DOCUMENT NUMBER: 98:53585  
 TITLE: High-pressure reactions of pyrroles with dimethyl  
 acetylenedicarboxylate  
 AUTHOR(S): Kotsuki, Hiyoshizo; Mori, Yuichiro; Nishizawa,  
 Hitoshi; Ochi, Masamitsu; Matsuoka, Kiyoshi  
 CORPORATE SOURCE: Fac. Sci., Kochi Univ., Kochi, 780, Japan  
 SOURCE: Heterocycles (1982), 19(10), 1915-20  
 CODEN: HTCYAM; ISSN: 0385-5414  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 OTHER SOURCE(S): CASREACT 98:53585  
 GI

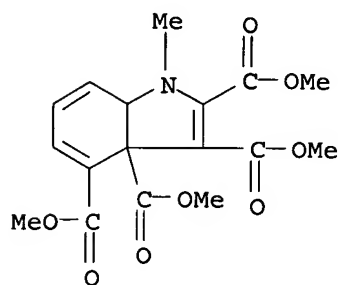


AB Treating pyrroles with  $\text{MeO}_2\text{CC} \cdot \text{tp} \cdot \text{bond} \cdot \text{CCO}_2\text{Me}$  (I) gave pyrroles II [R or R1 = H,  $\text{C}(\text{CO}_2\text{Me})\text{:CHCO}_2\text{Me}$ ], indole III, Diels-Alder adduct IV, and E- and Z-V. Thus, treating pyrrole with I at 15 kbar at 40° gave 16% E- and 2% Z-II [R = H, R1 =  $\text{C}(\text{CO}_2\text{Me})\text{:CHCO}_2\text{Me}$ ] and 3% II [R =  $\text{C}(\text{CO}_2\text{Me})\text{:CHCO}_2\text{Me}$ , R1 = H].

IT 1444-11-7P

RL: SPN (Synthetic preparation); PREP (Preparation)  
 (preparation of)

RN 1444-11-7 CAPLUS

CN 1H-Indole-2,3,3a,4(7aH)-tetracarboxylic acid, 1-methyl-, tetramethyl ester  
(9CI) (CA INDEX NAME)

L20 ANSWER 6 OF 9 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1976:121664 CAPLUS

DOCUMENT NUMBER: 84:121664

TITLE: Carboxylic acid amides

INVENTOR(S): Kabbe, Hans J.; Otten, Hinrich; Mayer, Karl Heinrich;  
Klauke, Erich

PATENT ASSIGNEE(S): Bayer A.-G., Fed. Rep. Ger.

SOURCE: Ger. Offen., 52 pp.

CODEN: GWXXBX

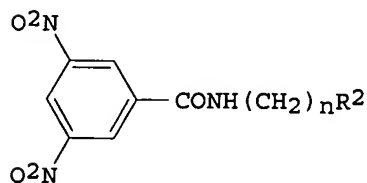
DOCUMENT TYPE: Patent

LANGUAGE: German

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 2428673	A1	19760102	DE 1974-2428673	19740614 <--
GB 1465255	A	19770223	GB 1975-20816	19750516 <--
US 3995044	A	19761130	US 1975-583464	19750603 <--
JP 51008262	A2	19760123	JP 1975-70276	19750612 <--
AT 7504510	A	19771115	AT 1975-4510	19750612 <--
BE 830211	A1	19751215	BE 1975-157305	19750613 <--
DK 7502680	A	19751215	DK 1975-2680	19750613 <--
NL 7507100	A	19751216	NL 1975-7100	19750613 <--
FR 2274294	A1	19760109	FR 1975-18588	19750613 <--
ES 438532	A1	19770201	ES 1975-438532	19750613 <--
PRIORITY APPLN. INFO.: GI			DE 1974-2428673	19740614



I

AB Amides RCONHR1 (R = substituted phenyl, R1 = heterocyclalkyl) (55  
compds.), including I (n = 1, R2 = 3-quinolyl, 3-pyridyl, 4-pyridyl,

6-methyl-2-pyridyl, 2-quinolyl, 2-pyridyl, 2-tetrahydrofuryl, 2,3-dihydro-4H-pyran-2-yl; n = 2, R2 = 2-pyridyl, n = 3, R2 = pyrrolo) were prepared by acylating R1NH2 with acid derivs. The amides are tuberculostatics. **Thus** I (n = 1, R2 = 2-pyridyl) had a min. inhibitory concentration against isoniazid-sensitive and -resistant

Mycobacterium

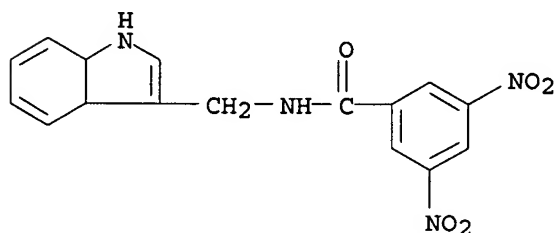
tuberculosis of 1 µg/ml.

IT 58624-84-3P

RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation of)

RN 58624-84-3 CAPLUS

CN Benzamide, N-(1H-indol-3-ylmethyl)-3,5-dinitro- (9CI) (CA INDEX NAME)



L20 ANSWER 7 OF 9 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1973:404733 CAPLUS

DOCUMENT NUMBER: 79:4733

TITLE: Thermal reorganization of select  
azabicyclo[m.n.0]nonatrienes. Generation of a  
cis,cis,trans,cis-azonine

AUTHOR(S): Anastassiou, A. G.; Elliott, R. L.; Wright, H. W.;  
Clardy, J.

CORPORATE SOURCE: Dep. Chem., Syracuse Univ., Syracuse, NY, USA  
SOURCE: Journal of Organic Chemistry (1973), 38(10),  
1959-61

CODEN: JOCEAH; ISSN: 0022-3263

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 79:4733

GI For diagram(s), see printed CA Issue.

AB Azabicyclononatriene (I) was warmed to 56° to give an equilibrium mixture of I and its isomer (II). At higher temps., i.e. 76°, two new isomers (III and IV) were formed. IV readily thermolyzes at 110° to yield a mixture of .apprx.35% III and 65% V. The reaction mechanism was examined by a cycloadditive trapping technique. **Thus**, I was treated with 2,5-dimethyl-3,4-diphenyl-2,4-cyclopentadienone to give azonine derivs. VI and VII. These products were explained in terms of the azonine intermediate (VIII).

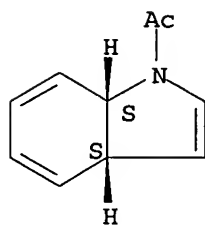
IT 41079-31-6P

RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation of)

RN 41079-31-6 CAPLUS

CN 1H-Indole, 1-acetyl-3a,7a-dihydro-, cis- (9CI) (CA INDEX NAME)

Relative stereochemistry.



L20 ANSWER 8 OF 9 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1965:90126 CAPLUS

DOCUMENT NUMBER: 62:90126

ORIGINAL REFERENCE NO.: 62:16021d-h

TITLE: Nuclear magnetic resonance spectra and conformations of 10-carbethoxy-1,1-dimethyldecalins. Conformational effects on proton nonequivalence

AUTHOR(S): Meyer, Walter L.; Davis, Daniel L.; Foster, Lincoln; Levinson, Alfred S.; Sawin, Virginia L.; Shew, D. Craig; Weddleton, Richard F.

CORPORATE SOURCE: Indiana Univ., Bloomington

SOURCE: Journal of the American Chemical Society (1965), 87(7), 1573-80

CODEN: JACSAT; ISSN: 0002-7863

DOCUMENT TYPE: Journal

LANGUAGE: English

GI For diagram(s), see printed CA Issue.

AB The O-methylene protons of the ethoxy groups in a series of 10-carbethoxy-1,1-dimethyl-trans-decalin and 10-carbethoxy-1,1-dimethyl-Δ8-octalinalone derivs. were magnetically nonequiv., proton magnetic resonance spectra of the Et groups being characteristic of ABC3 systems having chemical shifts of 0.07 to 0.16 ppm. between the methylene protons. Magnetic nonequivalence of the corresponding protons in an analogous series of 10-carbethoxy-trans-decalins and 10-carbethoxy-Δ8-octalinalones without 1,1-dimethyl substituents could not be detected, the ethoxyl resonances being of the A2B3 type in each case. From these results it is concluded that steric interaction between the ester and the axial 1β-Me group is of major importance in providing different magnetic environments for the O-methylene protons of the methylated derivs., probably due to depopulation of some otherwise accessible conformations of the ester group. Nonequivalence of the O-methylene protons of 10-carbethoxy-1,1-dimethyl-trans-2-decalone and 10-carbethoxy-1,1-dimethyl-Δ8-2-octalinalone could not be detected. Therefore it appears that in these 2 derivs., the only ones examined with 1,1-dimethyl substitution and trigonal hybridization at C-2, the gem-Me groups are differently oriented with respect to the ester than is the case for the other dimethylated compds., and that the methylated ring in such 2-ketones **thus** is not in a chair conformation. Synthesis of several of the substituted decalins is reported. Hydrogenation of I in acetic acid produces 1,1-dimethyl-2β-hydroxy-trans-decalin-10-carboxylic acid lactone. Successive saponification to the hydroxy acid, Jones oxidation to the oxo acid, and

ethylation afford the saturated keto ester II. That this in fact has a trans ring fusion is shown by its Wolff-Kishner reduction to the known 1,1-dimethyl-trans-decalin-10-carboxylic acid. 10-Carbethoxy-1,1-dimethyl-Δ8-octalinalone was prepared by conversion of the corresponding Δ8-7-ketone into its thioketal, followed by Raney nickel desulfurization. 10-Carbethoxy-Δ1.9-2-octalinalone,

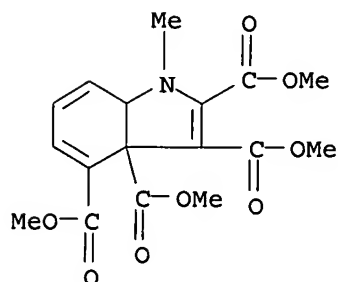
10-carbethoxy-trans-2-decalone, and I were converted into their thio ketals using the boron fluoride etherate technique.

IT 1444-11-7, Indole-2,3,3a,4(7aH)tetracarboxylic acid, 1-methyl-, tetramethyl ester

(nuclear magnetic resonance of)

RN 1444-11-7 CAPLUS

CN 1H-Indole-2,3,3a,4(7aH)-tetracarboxylic acid, 1-methyl-, tetramethyl ester (9CI) (CA INDEX NAME)



L20 ANSWER 9 OF 9 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1962:31317 CAPLUS

DOCUMENT NUMBER: 56:31317

ORIGINAL REFERENCE NO.: 56:5914d-g

TITLE: A new type of addition to 1-alkylpyrroles

AUTHOR(S): Acheson, R. M.; Hands, A. R.; Vernon, J. M.

CORPORATE SOURCE: Univ. Oxford, UK

SOURCE: Proc. Chem. Soc. (1961) 164-5

DOCUMENT TYPE: Journal

LANGUAGE: Unavailable

GI For diagram(s), see printed CA Issue.

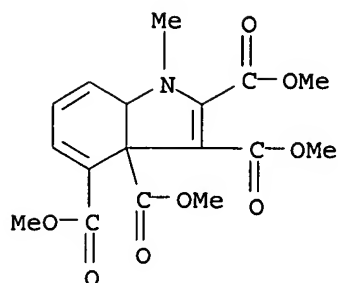
AB In the addition of (.tplbond.CCO2H)<sub>2</sub> to 1-benzylpyrrole, a minor product was the Diels-Alder adduct (I). With 1-methylpyrrole, (.tplbond.CCO2Me)<sub>2</sub> (II) gave a 2:1 adduct (III) as well as trimethyl 1-methylpyrrole-2,3,4-tricarboxylate (IV). III heated with II gave IV and vic-C<sub>6</sub>H<sub>3</sub>(CO<sub>2</sub>Me)<sub>3</sub> (V). IV was hydrolyzed to a tricarboxylic acid, which selectively lost CO<sub>2</sub> from the 2- and 3-positions to give 1-methylindole-4-carboxylic acid. Thus, the 2:1 adduct could be formulated as shown. III was probably formed by Diels-Alder addition of II to 1-methylpyrrole to give a 1:1 adduct, which reacted with a 2nd mol. of the ester. The loss of one ester group on aromatization, the formation of IV and V by addition of II across the 4,7-positions of the adduct, and the scission of the resulting mol. were now understandable.

IT 1444-11-7, Indole-2,3,3a,4(7aH)tetracarboxylic acid, 1-methyl-, tetramethyl ester

(preparation of)

RN 1444-11-7 CAPLUS

CN 1H-Indole-2,3,3a,4(7aH)-tetracarboxylic acid, 1-methyl-, tetramethyl ester (9CI) (CA INDEX NAME)



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SINCE FILE	TOTAL
ENTRY	SESSION
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DICTIONARY FILE UPDATES: 21 JUN 2004 HIGHEST RN 697224-75-2

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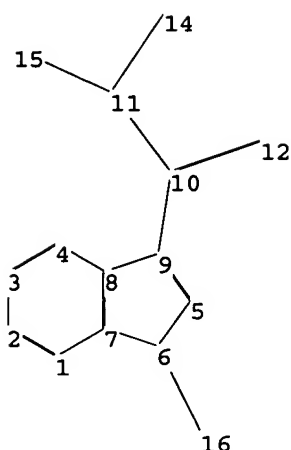
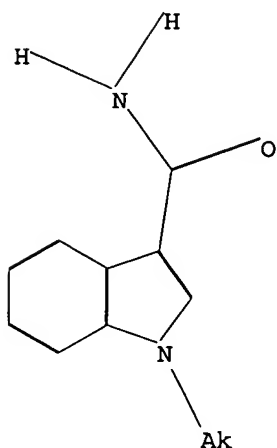
Experimental and calculated property data are now available. For more information enter HELP PROP at an arrow prompt in the file or refer to the file summary sheet on the web at:

<http://www.cas.org/ONLINE/DBSS/registryss.html>

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```

chain nodes :
10 11 12 14 15 16
ring nodes :
1 2 3 4 5 6 7 8 9
chain bonds :
6-16 9-10 10-11 10-12 11-14 11-15
ring bonds :
1-2 1-7 2-3 3-4 4-8 5-6 5-9 6-7 7-8 8-9
exact/norm bonds :
5-6 6-7 6-16 10-11 10-12
exact bonds :
5-9 8-9 9-10 11-14 11-15
normalized bonds :
1-2 1-7 2-3 3-4 4-8 7-8
isolated ring systems :
containing 1 :

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Match level :

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1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:CLASS
11:CLASS 12:CLASS 14:CLASS 15:CLASS 16:CLASS

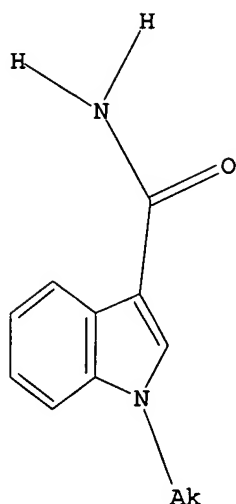
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L21 STRUCTURE UPLOADED

=> d 121

L21 HAS NO ANSWERS

L21 STR



Structure attributes must be viewed using STN Express query preparation.

=> s l21

SAMPLE SEARCH INITIATED 12:13:18 FILE 'REGISTRY'  
SAMPLE SCREEN SEARCH COMPLETED - 522 TO ITERATE

100.0% PROCESSED 522 ITERATIONS  
SEARCH TIME: 00.00.01

4 ANSWERS

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*  
BATCH \*\*COMPLETE\*\*  
PROJECTED ITERATIONS: 9070 TO 11810  
PROJECTED ANSWERS: 4 TO 200

L22 4 SEA SSS SAM L21

=> s l21 sss full

FULL SEARCH INITIATED 12:13:32 FILE 'REGISTRY'  
FULL SCREEN SEARCH COMPLETED - 10087 TO ITERATE

100.0% PROCESSED 10087 ITERATIONS  
SEARCH TIME: 00.00.01

58 ANSWERS

L23 58 SEA SSS FUL L21

FIL CAPLUS  
COST IN U.S. DOLLARS

SINCE FILE ENTRY	TOTAL SESSION
155.42	990.42

FULL ESTIMATED COST

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE ENTRY	TOTAL SESSION
0.00	-6.24

CA SUBSCRIBER PRICE

FILE 'CAPLUS' ENTERED AT 12:13:45 ON 22 JUN 2004  
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10714568

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FILE COVERS 1907 - 22 Jun 2004 VOL 140 ISS 26  
FILE LAST UPDATED: 21 Jun 2004 (20040621/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s l23

L24 37 L23

=> s l24 and py<=2002

22503583 PY<=2002

L25 33 L24 AND PY<=2002

=> s l25 and thu

138 THU

2162536 THUS

2162659 THU

(THU OR THUS)

L26 6 L25 AND THU

=> s l25 p/dt

MISSING OPERATOR L25 P/DT

The search profile that was entered contains terms or nested terms that are not separated by a logical operator.

=> s l25 and p/dt

4372814 P/DT

L27 11 L25 AND P/DT

=> d his

(FILE 'HOME' ENTERED AT 11:53:52 ON 22 JUN 2004)

FILE 'REGISTRY' ENTERED AT 11:54:22 ON 22 JUN 2004

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L3	0 S L1 SSS FULL
L4	STRUCTURE UPLOADED
L5	0 S L4
L6	0 S L4 SSS FULL
L7	STRUCTURE UPLOADED
L8	0 S L7
L9	0 S L7 SSS FULL
L10	STRUCTURE UPLOADED
L11	1 S L10
L12	1 S L10 SSS FULL

10714568

06/22/2004

FILE 'CAPLUS' ENTERED AT 12:01:50 ON 22 JUN 2004

L13 0 S L12  
L14 0 S L12

FILE 'REGISTRY' ENTERED AT 12:06:06 ON 22 JUN 2004

L15 STRUCTURE UPLOADED  
L16 2 S L15  
L17 89 S L15 SSS FULL

FILE 'CAPLUS' ENTERED AT 12:06:39 ON 22 JUN 2004

L18 34 S L17  
L19 29 S L18 AND PY<=2002  
L20 9 S L19 AND THU

FILE 'REGISTRY' ENTERED AT 12:12:57 ON 22 JUN 2004

L21 STRUCTURE UPLOADED  
L22 4 S L21  
L23 58 S L21 SSS FULL

FILE 'CAPLUS' ENTERED AT 12:13:45 ON 22 JUN 2004

L24 37 S L23  
L25 33 S L24 AND PY<=2002  
L26 6 S L25 AND THU  
L27 11 S L25 AND P/DT

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L26 ANSWER 1 OF 6 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 2002:213824 CAPLUS

DOCUMENT NUMBER: 136:247492

TITLE: Preparation of indolecarboxylates as neoplasm inhibitors.

INVENTOR(S): Pamukcu, Rifat; Piazza, Gary A.

PATENT ASSIGNEE(S): Cell Pathways, Inc., USA

SOURCE: U.S., 45 pp., Cont. of U.S. Ser. No. 200,139, abandoned.

CODEN: USXXAM

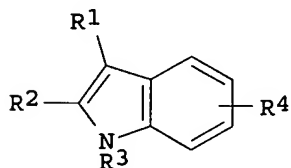
DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 6358992	B1	20020319	US 1999-443395	19991119 <--
PRIORITY APPLN. INFO.:			US 1998-200139	B1 19981125
OTHER SOURCE(S):		MARPAT 136:247492		
GI				



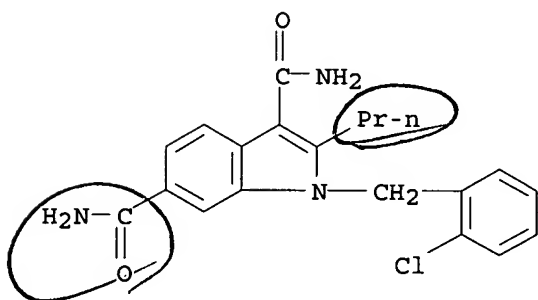
I

AB Claimed is a method of treating a mammal having precancerous lesions comprising administration of title compds. [I; R1 = H, halo, NO<sub>2</sub>, (protected) carboxy, acyl, cyano, hydroxyiminoalkyl, alkenyl optionally substituted with oxo, alkyl optionally substituted with protected carboxy, carboxy, OH; R2 = H, halo, alkenyl, acyl, alkyl optionally substituted with protected carboxy, carboxy, alkoxy, OH; R1R2 = atoms to form a 4-7 membered (oxo)carbocyclic ring; R3 = (substituted) alkenyl, alkyl; R4 = (protected) carboxy, acyl, cyano, halo, heterocyclyl, amino optionally substituted with acyl or protected carboxy, alkyl optionally substituted with (protected) carboxy, acyl] (no data). Thus, Me 3-acetyl-2-propylindole-6-carboxylate in DMF was treated with NaH then with 2-chlorobenzyl bromide followed by stirring for 1 h to give Me 3-acetyl-1-(2-chlorobenzyl)-2-propylindole-6-carboxylate.

IT 184150-24-1P  
 RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)  
 (preparation of indolecarboxylates as neoplasm inhibitors)

RN 184150-24-1 CAPLUS

CN 1H-Indole-3,6-dicarboxamide, 1-[(2-chlorophenyl)methyl]-2-propyl- (9CI)  
 (CA INDEX NAME)



REFERENCE COUNT: 17 THERE ARE 17 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L26 ANSWER 2 OF 6 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 2001:597959 CAPLUS

DOCUMENT NUMBER: 135:166782

TITLE: Solid-phase process for making indole compounds

INVENTOR(S): Ketcha, Daniel Michael; Wilson, Lawrence Joseph

PATENT ASSIGNEE(S): Procter + Gamble Co., USA

SOURCE: PCT Int. Appl., 13 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

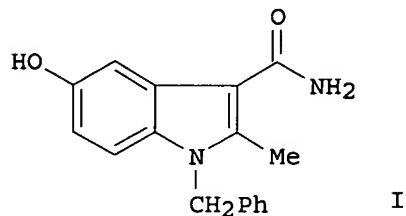
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001058870	A2	<del>20010816</del>	WO 2001-US4216	20010208 <--
WO 2001058870	A3	20020404		

W: AE, AG, AL, AM, AT, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, CZ, DE, DE, DK, DK, DM, DZ, EE, EE, ES, FI, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SK, SL, TJ, TM, TR,

06/22/2004

TT, TZ, UA, UG, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU,  
 TJ, TM  
 RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY,  
 DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF,  
 BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG

US 2002002286 A1 20020103 US 2001-779080 20010208 <--  
 PRIORITY APPLN. INFO.: US 2000-181155P P 20000209  
 OTHER SOURCE(S): CASREACT 135:166782; MARPAT 135:166782  
 GI



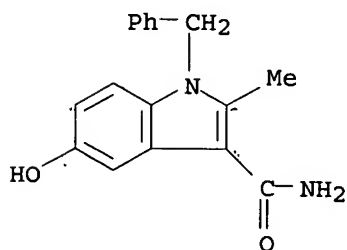
AB Indole compds., e.g. I, were prepared by a solid-phase process. The process was comprised of the following steps: (a) deprotection and treatment of ArgoPore-Rink-NH-Fmoc resin with diketene to provide a resin-bound acetoacetamide; (b) treating the product from Step (a) with a primary amine in the presence of a dehydrating agent to provide a resin-bound enaminone; (c) treating the product from Step (b) with a 1,4-benzoquinone, and releasing the resulting indole product from the resin. **Thus**, I and related derivs. were produced in 5 steps from ArgoPore-Rink-NH-Fmoc resin.

IT 302598-58-9P 302598-59-0P 302598-60-3P  
 302598-61-4P 302598-62-5P 302598-63-6P  
 302598-65-8P 302598-66-9P 302598-67-0P  
 302598-68-1P 302598-69-2P 302598-70-5P  
 302598-71-6P 354137-88-5P

RL: IMF (Industrial manufacture); SPN (Synthetic preparation); PREP (Preparation)  
 (solid-phase process for making indole compds.)

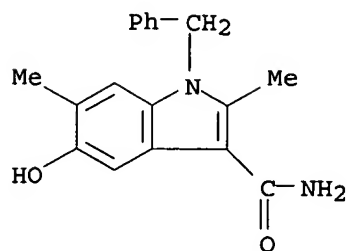
RN 302598-58-9 CAPLUS

CN 1H-Indole-3-carboxamide, 5-hydroxy-2-methyl-1-(phenylmethyl)- (9CI) (CA INDEX NAME)

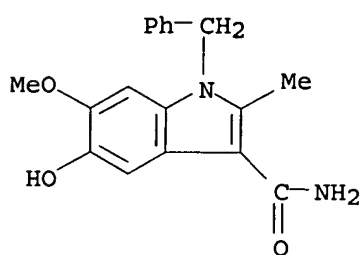


RN 302598-59-0 CAPLUS

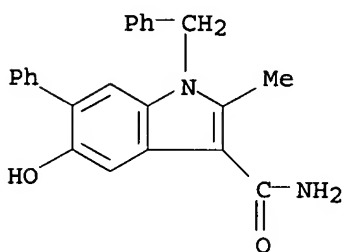
CN 1H-Indole-3-carboxamide, 5-hydroxy-2,6-dimethyl-1-(phenylmethyl)- (9CI) (CA INDEX NAME)



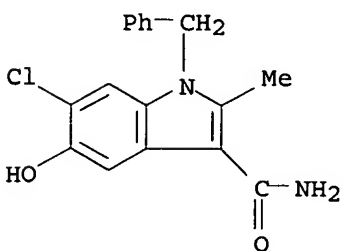
RN 302598-60-3 CAPLUS

CN 1H-Indole-3-carboxamide, 5-hydroxy-6-methoxy-2-methyl-1-(phenylmethyl)-  
(9CI) (CA INDEX NAME)

RN 302598-61-4 CAPLUS

CN 1H-Indole-3-carboxamide, 5-hydroxy-2-methyl-6-phenyl-1-(phenylmethyl)-  
(9CI) (CA INDEX NAME)

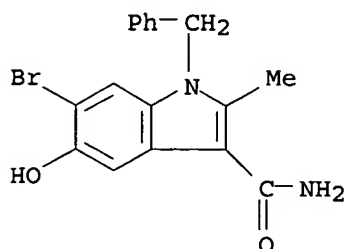
RN 302598-62-5 CAPLUS

CN 1H-Indole-3-carboxamide, 6-chloro-5-hydroxy-2-methyl-1-(phenylmethyl)-  
(9CI) (CA INDEX NAME)

RN 302598-63-6 CAPLUS

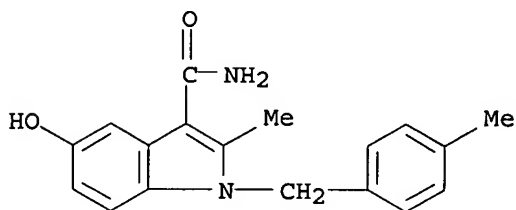
10714568

CN 1H-Indole-3-carboxamide, 6-bromo-5-hydroxy-2-methyl-1-(phenylmethyl)-  
(9CI) (CA INDEX NAME)



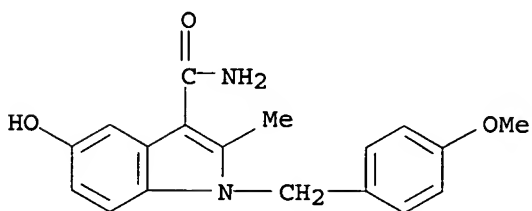
RN 302598-65-8 CAPLUS

CN 1H-Indole-3-carboxamide, 5-hydroxy-2-methyl-1-[(4-methylphenyl)methyl]-  
(9CI) (CA INDEX NAME)



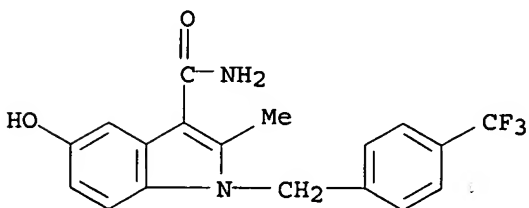
RN 302598-66-9 CAPLUS

CN 1H-Indole-3-carboxamide, 5-hydroxy-1-[(4-methoxyphenyl)methyl]-2-methyl-  
(9CI) (CA INDEX NAME)



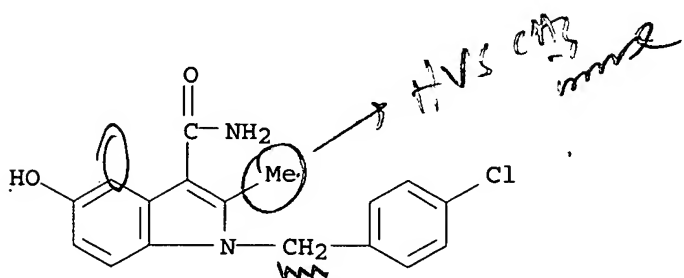
RN 302598-67-0 CAPLUS

CN 1H-Indole-3-carboxamide, 5-hydroxy-2-methyl-1-[[4-(trifluoromethyl)phenyl]methyl]- (9CI) (CA INDEX NAME)

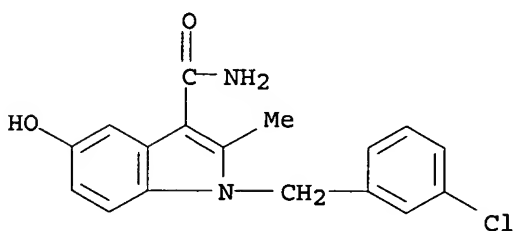




RN 302598-68-1 CAPLUS

CN 1H-Indole-3-carboxamide, 1-[(4-chlorophenyl)methyl]-5-hydroxy-2-methyl-  
(9CI) (CA INDEX NAME)

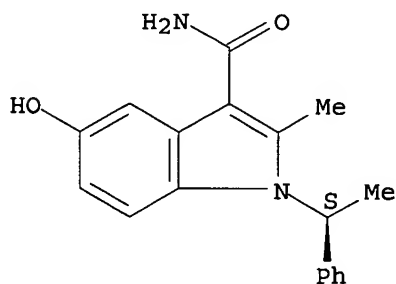
RN 302598-69-2 CAPLUS

CN 1H-Indole-3-carboxamide, 1-[(3-chlorophenyl)methyl]-5-hydroxy-2-methyl-  
(9CI) (CA INDEX NAME)

RN 302598-70-5 CAPLUS

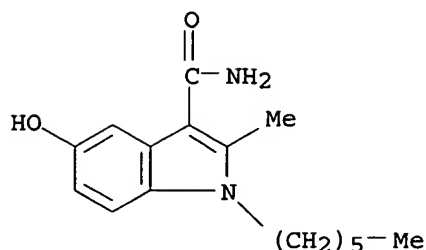
CN 1H-Indole-3-carboxamide, 5-hydroxy-2-methyl-1-[(1S)-1-phenylethyl]- (9CI)  
(CA INDEX NAME)

Absolute stereochemistry.



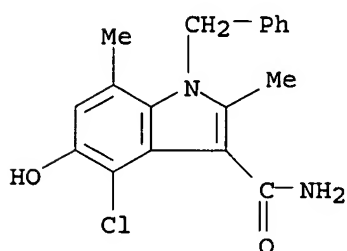
RN 302598-71-6 CAPLUS

CN 1H-Indole-3-carboxamide, 1-hexyl-5-hydroxy-2-methyl- (9CI) (CA INDEX  
NAME)



RN 354137-88-5 CAPLUS

CN 1H-Indole-3-carboxamide, 4-chloro-5-hydroxy-2,7-dimethyl-1-(phenylmethyl)-(9CI) (CA INDEX NAME)



L26 ANSWER 3 OF 6 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1997:513631 CAPLUS

DOCUMENT NUMBER: 127:205572

TITLE: Preparation of thiazolylbenzofurans as leukotriene and SRS-A antagonists or inhibitors

INVENTOR(S): Matsuo, Masaaki; Okumura, Kazuo; Shigenaga, Shinji; Nishimura, Hiroaki; Matsuda, Hiroshi; Hagiwara, Daijiro; Terasaka, Tadashi

PATENT ASSIGNEE(S): Fujisawa Pharmaceutical Co., Ltd., Japan

SOURCE: PCT Int. Appl., 244 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

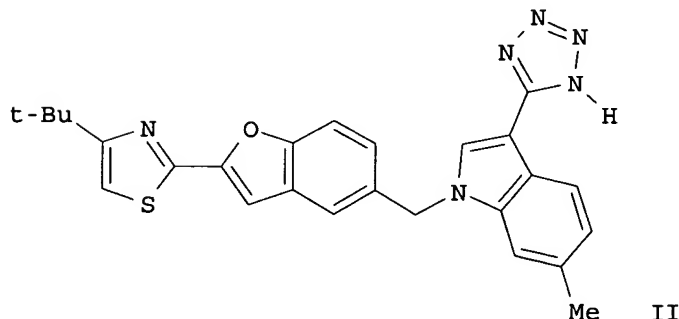
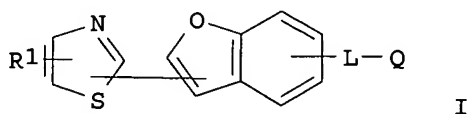
LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

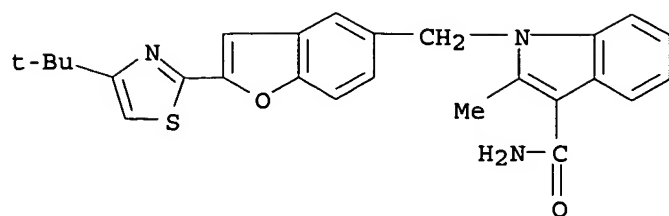
PATENT INFORMATION:

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WO 9727190	A1	19970731	WO 1997-JP73	19970117 <--
W: AU, CA, CN, HU, JP, KR, MX, SG, US, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
ZA 9700415	A	19970730	ZA 1997-415	19970117 <--
CA 2244189	AA	19970731	CA 1997-2244189	19970117 <--
AU 9713991	A1	19970820	AU 1997-13991	19970117 <--
EP 880519	A1	19981202	EP 1997-900432	19970117 <--
EP 880519	B1	20020417		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, PT, IE, FI				
CN 1209809	A	19990303	CN 1997-191798	19970117 <--
JP 2000503984	T2	20000404	JP 1997-526720	19970117 <--
EP 1170009	A2	20020109	EP 2001-123263	19970117 <--

EP 1170009 A3 20020116  
 EP 1170009 B1 20040407  
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 TW 474811 B 20020201 TW 1997-86100473 19970117 <--  
 AT 216384 E 20020515 AT 1997-900432 19970117 <--  
 ES 2171878 T3 20020916 ES 1997-900432 19970117 <--  
 AT 263561 E 20040415 AT 2001-123263 19970117  
 US 5994378 A 19991130 US 1998-101766 19980721 <--  
 PRIORITY APPLN. INFO.: GB 1996-1235 A 19960122  
 AU 1996-1111 A 19960718  
 AU 1996-9241 A 19960412  
 EP 1997-900432 A3 19970117  
 WO 1997-JP73 W 19970117  
 OTHER SOURCE(S): MARPAT 127:205572  
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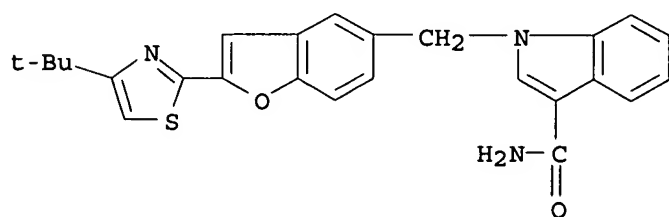


- AB The title compds. [I; R1 = lower alkyl; L = single bond, (un)substituted lower alkylene; Q = (un)substituted heterocyclic group, lower alkoxy substituted with aryl] which possess activities as leukotriene and SRS-A antagonists or inhibitors, and are useful in the treatment and/or prevention of allergy or inflammation, were prepared **Thus**, treatment of 4-tert-butyl-2-{5-[(3-cyano-6-methylindol-1-yl)methyl]benzofuran-2-yl}thiazole with NaN<sub>3</sub> and NH<sub>4</sub>Cl in DMF afforded the title compound II which showed IC<sub>50</sub> of < 5 nM against 3H-leukotriene D<sub>4</sub> receptor binding.
- IT **194488-60-3P 194488-61-4P**  
 RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)  
 (preparation of thiazolylbenzofurans as leukotriene and SRS-A antagonists or inhibitors)
- RN 194488-60-3 CAPLUS  
 CN 1H-Indole-3-carboxamide, 1-[[2-[4-(1,1-dimethylethyl)-2-thiazolyl]-5-benzofuranyl]methyl]-2-methyl- (9CI) (CA INDEX NAME)



RN 194488-61-4 CAPLUS

CN 1H-Indole-3-carboxamide, 1-[[2-[4-(1,1-dimethylethyl)-2-thiazolyl]-5-benzofuranyl]methyl]- (9CI) (CA INDEX NAME)



L26 ANSWER 4 OF 6 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1994:483050 CAPLUS

DOCUMENT NUMBER: 121:83050

TITLE: Preparation of 2-indolinethiones and related disulfides and seleno-analogs as protein tyrosine kinase inhibitors and antitumor agents

INVENTOR(S): Dobrusin, Ellen Myra; Showalter, Howard Daniel Hollis; Denny, William Alexander; Palmer, Brian Desmond; Rewcastle, Gordon William; Tercel, Moana; Thompson, Andrew Mark

PATENT ASSIGNEE(S): Warner-Lambert Co., USA

SOURCE: PCT Int. Appl., 212 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 2

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9403427	A1	19940217	WO 1993-US7272	19930802 <--
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RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
EP 654024	A1	19950524	EP 1993-918594	19930802 <--
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, MC, NL, PT, SE				
HU 71553	A2	19951228	HU 1995-341	19930802 <--
JP 08503450	T2	19960416	JP 1993-519671	19930802 <--
AU 672224	B2	19960926	AU 1993-47994	19930802 <--
AU 9347994	A1	19940303		
CZ 283965	B6	19980715	CZ 1995-288	19930802 <--
NZ 255194	A	20000128	NZ 1993-255194	19930802 <--
RU 2155187	C2	20000827	RU 1995-108332	19930802 <--
SK 283413	B6	20030701	SK 1995-135	19930802

06/22/2004

PRIORITY APPLN. INFO.:

US 1992-926015

A 19920806

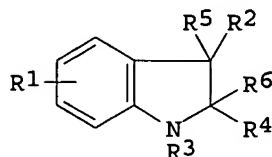
WO 1993-US7272

W 19930802

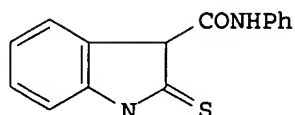
OTHER SOURCE(S):

MARPAT 121:83050

GI



I



II

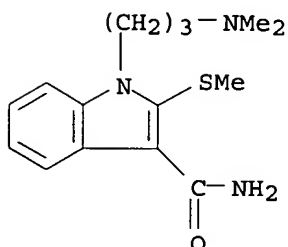
AB Title compds. [I; R1 = H, halo, OH, alkyl, alkoxy, CO2H, etc.; 1 or 2 CR1 = N; R2 = (acyl)alkyl, CH:CHCO2H, alkylcarbonyl, acyl, etc.; R3 = H, alkyl, CH2Ph; R4 = ZH, ZnX, ZnQ; R5 = H and R4R6 = S or Se; R5R6 = bond; Q = I in which R4 = Zn and R5R6 = bond; X = H, alkyl, CH2Ph, (hetero)aryl; Z = S, Se; n = 0-3] were prepared Thus, 1-methyl-2-indolinone was treated with P2S5 and the product treated with NaH and PhNCO to give indolinethionecarboxamide II which had IC50 of 2μM against epidermal growth factor mediated mitogenesis.

IT 156137-01-8P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
(preparation and reaction of, in preparation of protein tyrosine kinase inhibitor)

RN 156137-01-8 CAPLUS

CN 1H-Indole-3-carboxamide, 1-[3-(dimethylamino)propyl]-2-(methylthio)- (9CI)  
(CA INDEX NAME)



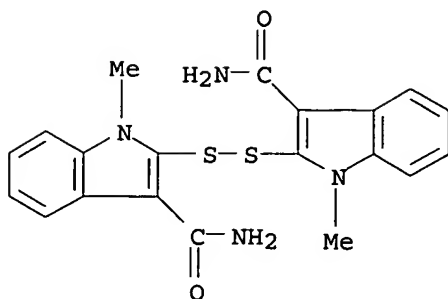
IT 156136-31-1P

RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation of, as protein tyrosine kinase inhibitor)

RN 156136-31-1 CAPLUS

CN 1H-Indole-3-carboxamide, 2,2'-dithiobis[1-methyl- (9CI) (CA INDEX NAME)

103



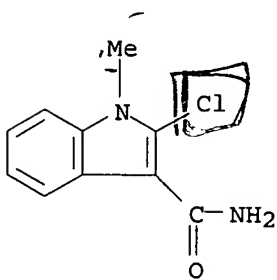
IT 120110-10-3

RL: RCT (Reactant); RACT (Reactant or reagent)

(reaction of, in preparation of protein tyrosine kinase inhibitor)

RN 120110-10-3 CAPLUS

CN 1H-Indole-3-carboxamide, 2-chloro-1-methyl- (9CI) (CA INDEX NAME)



L26 ANSWER 5 OF 6 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1991:163923 CAPLUS

DOCUMENT NUMBER: 114:163923

TITLE: First reactions of vinylindoles with diethyl mesoxalate, nitrosobenzene, and chlorosulfonyl isocyanate: new functionalized and [b]annulated indoles

AUTHOR(S): Pindur, Ulf; Kim, Myung Hwa

CORPORATE SOURCE: Inst. Pharm., Univ. Mainz, Mainz, D-6500, Fed. Rep. Ger.

SOURCE: Tetrahedron (1989), 45(20), 6427-38

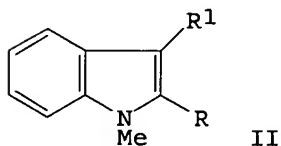
CODEN: TETRAB; ISSN: 0040-4020

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 114:163923

GI



II

AB Di-Et mesoxalate (I) reacts with 2- and 3-vinylindoles via electrophilic

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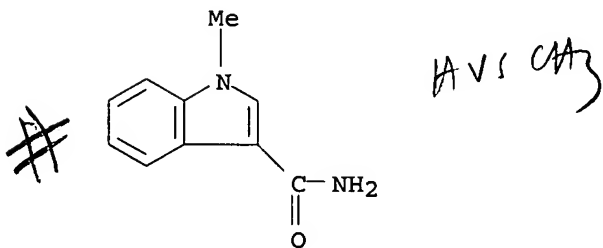
substitution to give new, functionalized and annulated indoles with high regioselectivity. Thus, vinylindoles II (R = CH:CHR<sub>2</sub>, R<sub>1</sub> = H; R<sub>2</sub> = Me, CO<sub>2</sub>Me) reacted with I to give II [R<sub>1</sub> = C(OH)(CO<sub>2</sub>Me)<sub>2</sub>]. Regio-controlled dimerization processes occur in the reactions of the vinylindoles II (R = CH:CHMe, R<sub>1</sub> = H; R = H, R<sub>1</sub> = CH:CH<sub>2</sub>). Nitrosobenzene reacts with 2- and 3-vinylindoles in a multi-stage sequence including regiospecific tandem hetero-Diels-Alder reactions and cycloreversions to give the new, 2,3-difunctionalized indoles II (R = CH:NPh, R<sub>1</sub> = NPhOH; R = NPhOH, R<sub>1</sub> = CH:NPh), which are conformationally stabilized by proton chelation. The heterocumulene chlorosulfonyl isocyanate reacts as a simple electrophile (like di-Et mesoxalate) with 2-vinylindole II (R = CH:CHCO<sub>2</sub>Me, R<sub>1</sub> = H) to give the indole-3-carboxamide II (R same, R<sub>1</sub> = CONH<sub>2</sub>). In addition, analogous reactions of N-methylindole were also studied and, in most cases, gave comparable reactivity patterns.

IT 118959-44-7P 127744-56-3P

RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation of)

RN 118959-44-7 CAPLUS

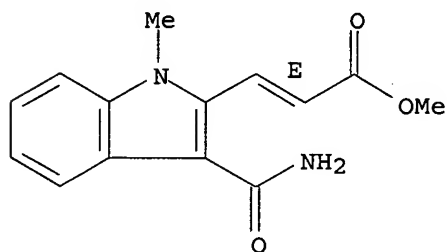
CN 1H-Indole-3-carboxamide, 1-methyl- (9CI) (CA INDEX NAME)



RN 127744-56-3 CAPLUS

CN 2-Propenoic acid, 3-[3-(aminocarbonyl)-1-methyl-1H-indol-2-yl]-, methyl ester, (E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



L26 ANSWER 6 OF 6 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1990:552390 CAPLUS

DOCUMENT NUMBER: 113:152390

TITLE: Preparation of spirocyclic compounds incorporating five-membered rings with two heteroatoms, especially spiro[azabicyclooctanoxazoles], useful as drugs

INVENTOR(S): Baker, Raymond; Kneen, Clare O.; Saunders, John; Swain, Christopher

PATENT ASSIGNEE(S): Merck Sharp and Dohme Ltd., UK

SOURCE: Eur. Pat. Appl., 38 pp.

10714568

CODEN: EPXXDW  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 337547	A1	19891018	EP 1989-200862	19890406 <--
EP 337547	B1	19940302		
R: AT, BE, CH, DE, ES, FR, GB, GR, IT, LI, LU, NL, SE				
FI 8901584	A	19891012	FI 1989-1584	19890403 <--
US 4940703	A	19900710	US 1989-333076	19890404 <--
AT 102205	E	19940315	AT 1989-200862	19890406 <--
ES 2061933	T3	19941216	ES 1989-200862	19890406 <--
AU 8932632	A1	19891012	AU 1989-32632	19890410 <--
AU 617785	B2	19911205		
DK 8901704	A	19891012	DK 1989-1704	19890410 <--
NO 8901471	A	19891012	NO 1989-1471	19890410 <--
JP 01305092	A2	19891208	JP 1989-88177	19890410 <--
ZA 8902587	A	19900328	ZA 1989-2587	19890410 <--
PRIORITY APPLN. INFO.:			GB 1988-8433	19880411
			EP 1989-200862	19890406

OTHER SOURCE(S): MARPAT 113:152390

GI For diagram(s), see printed CA Issue.

AB Title compds. I [R1 = H, OH, alkyl, alkenyl, alkynyl, alkoxy, PhCH2O, hydroxyalkyl, halo, amino, cyano, NO2, (substituted) carbamoyl or sulfamoyl; R2 = H, halo, alkyl, alkoxy, alkylcarbonyl; V = N, CH, C; W = O, S, (substituted) NH; 2 of X, Y, Z = O, S, N; other = C; or Y = CO; Q = residue of aza(bi)cyclic system], some of which act on 5-HT3 receptors (no data), are prepared for treatment of psychosis, anxiety, gastric dysfunction, nausea, senile dementia, etc. **Thus**, treatment of 1-methyl-1H-indole-3-nitrile with dry HCl in MeOH gave the Me imidate HCl salt, which underwent cyclocondensation with 3-aminomethyl-3-hydroxy-1-azabicyclo[2.2.2]octane di-HCl in refluxing MeOH to give, after acidification, (methylinolyl)spiro[azabicyclooctanoxazole] II as the di-HCl salt.

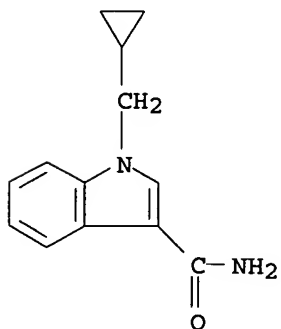
IT 128200-23-7P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and reaction of, in preparation of serotoninergic S3 antagonists)

RN 128200-23-7 CAPLUS

CN 1H-Indole-3-carboxamide, 1-(cyclopropylmethyl)- (9CI) (CA INDEX NAME)



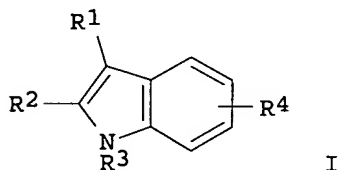


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L27 ANSWER 1 OF 11 CAPLUS COPYRIGHT 2004 ACS on STN  
 ACCESSION NUMBER: 2002:213824 CAPLUS  
 DOCUMENT NUMBER: 136:247492  
 TITLE: Preparation of indolecarboxylates as neoplasm inhibitors.  
 INVENTOR(S): Pamukcu, Rifat; Piazza, Gary A.  
 PATENT ASSIGNEE(S): Cell Pathways, Inc., USA  
 SOURCE: U.S., 45 pp., Cont. of U.S. Ser. No. 200,139, abandoned.  
 CODEN: USXXAM  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 6358992	B1	20020319	US 1999-443395	19991119 <--
PRIORITY APPLN. INFO.:			US 1998-200139	B1 19981125
OTHER SOURCE(S):		MARPAT 136:247492		

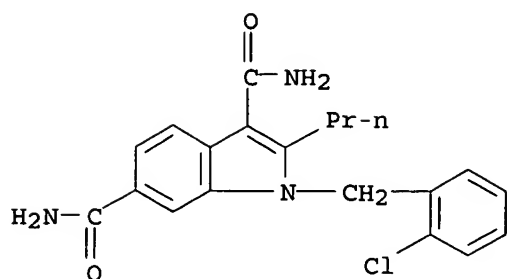
GI



AB Claimed is a method of treating a mammal having precancerous lesions comprising administration of title compds. [I; R1 = H, halo, NO<sub>2</sub>, (protected) carboxy, acyl, cyano, hydroxyiminoalkyl, alkenyl optionally substituted with oxo, alkyl optionally substituted with protected carboxy, carboxy, OH; R2 = H, halo, alkenyl, acyl, alkyl optionally substituted with protected carboxy, carboxy, alkoxy, OH; R1R2 = atoms to form a 4-7 membered (oxo)carbocyclic ring; R3 = (substituted) alkenyl, alkyl; R4 = (protected) carboxy, acyl, cyano, halo, heterocyclyl, amino optionally substituted with acyl or protected carboxy, alkyl optionally substituted with (protected) carboxy, acyl] (no data). Thus, Me 3-acetyl-2-propylindole-6-carboxylate in DMF was treated with NaH then with 2-chlorobenzyl bromide followed by stirring for 1 h to give Me 3-acetyl-1-(2-chlorobenzyl)-2-propylindole-6-carboxylate.

IT 184150-24-1P  
 RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)  
 (preparation of indolecarboxylates as neoplasm inhibitors)

RN 184150-24-1 CAPLUS  
 CN 1H-Indole-3,6-dicarboxamide, 1-[(2-chlorophenyl)methyl]-2-propyl- (9CI)  
 (CA INDEX NAME)



REFERENCE COUNT: 17 THERE ARE 17 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L27 ANSWER 2 OF 11 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 2001:597959 CAPLUS

DOCUMENT NUMBER: 135:166782

TITLE: Solid-phase process for making indole compounds

INVENTOR(S): Ketcha, Daniel Michael; Wilson, Lawrence Joseph

PATENT ASSIGNEE(S): Procter + Gamble Co., USA

SOURCE: PCT Int. Appl., 13 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

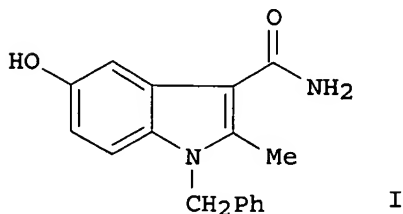
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001058870	A2	20010816	WO 2001-US4216	20010208 <--
WO 2001058870	A3	20020404		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
US 2002002286	A1	20020103	US 2001-779080	20010208 <--

PRIORITY APPLN. INFO.: US 2000-181155P P 20000209

OTHER SOURCE(S): CASREACT 135:166782; MARPAT 135:166782

GI



AB Indole compds., e.g. I, were prepared by a solid-phase process. The process was comprised of the following steps: (a) deprotection and treatment of ArgoPore-Rink-NH-Fmoc resin with diketene to provide a resin-bound acetoacetamide; (b) treating the product from Step (a) with a primary amine in the presence of a dehydrating agent to provide a resin-bound enaminone; (c) treating the product from Step (b) with a 1,4-benzoquinone, and releasing the resulting indole product from the resin. Thus, I and related derivs. were produced in 5 steps from ArgoPore-Rink-NH-Fmoc resin.

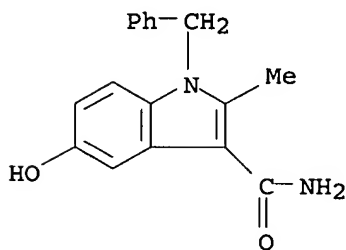
IT 302598-58-9P 302598-59-0P 302598-60-3P  
 302598-61-4P 302598-62-5P 302598-63-6P  
 302598-65-8P 302598-66-9P 302598-67-0P  
 302598-68-1P 302598-69-2P 302598-70-5P  
 302598-71-6P 354137-88-5P

RL: IMF (Industrial manufacture); SPN (Synthetic preparation); PREP (Preparation)

(solid-phase process for making indole compds.)

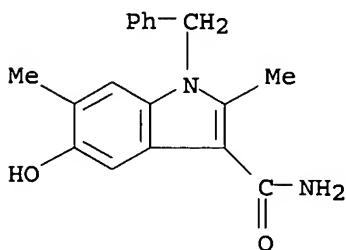
RN 302598-58-9 CAPLUS

CN 1H-Indole-3-carboxamide, 5-hydroxy-2-methyl-1-(phenylmethyl)- (9CI) (CA INDEX NAME)



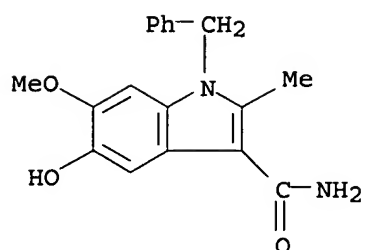
RN 302598-59-0 CAPLUS

CN 1H-Indole-3-carboxamide, 5-hydroxy-2,6-dimethyl-1-(phenylmethyl)- (9CI) (CA INDEX NAME)

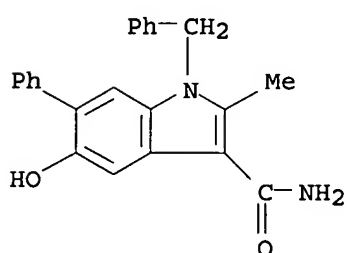


RN 302598-60-3 CAPLUS

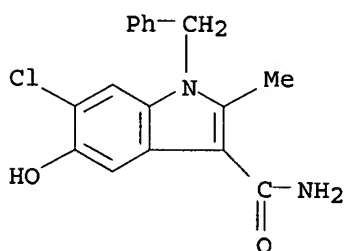
CN 1H-Indole-3-carboxamide, 5-hydroxy-6-methoxy-2-methyl-1-(phenylmethyl)- (9CI) (CA INDEX NAME)



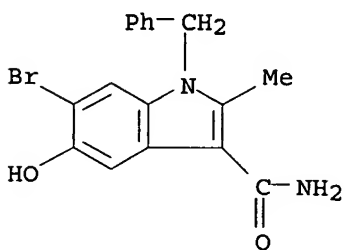
RN 302598-61-4 CAPLUS

CN 1H-Indole-3-carboxamide, 5-hydroxy-2-methyl-6-phenyl-1-(phenylmethyl)-  
(9CI) (CA INDEX NAME)

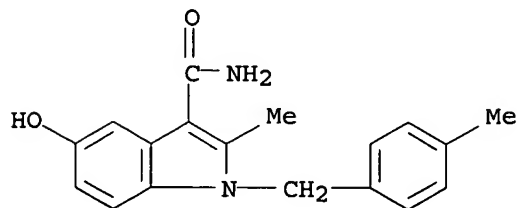
RN 302598-62-5 CAPLUS

CN 1H-Indole-3-carboxamide, 6-chloro-5-hydroxy-2-methyl-1-(phenylmethyl)-  
(9CI) (CA INDEX NAME)

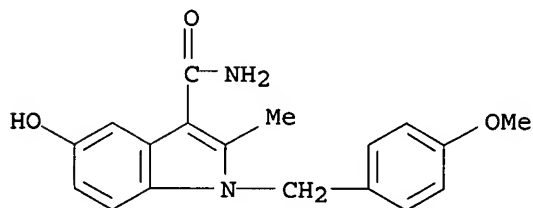
RN 302598-63-6 CAPLUS

CN 1H-Indole-3-carboxamide, 6-bromo-5-hydroxy-2-methyl-1-(phenylmethyl)-  
(9CI) (CA INDEX NAME)

RN 302598-65-8 CAPLUS

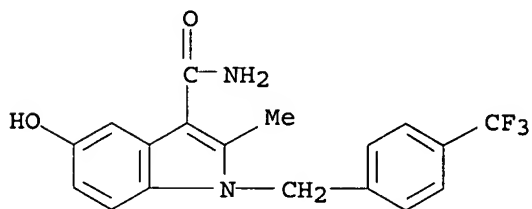
CN 1H-Indole-3-carboxamide, 5-hydroxy-2-methyl-1-[(4-methylphenyl)methyl]-  
(9CI) (CA INDEX NAME)

RN 302598-66-9 CAPLUS

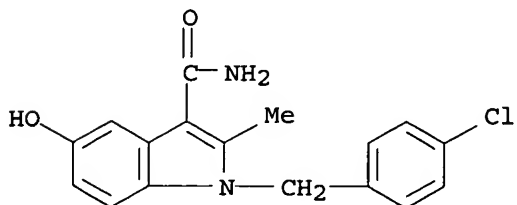
CN 1H-Indole-3-carboxamide, 5-hydroxy-1-[(4-methoxyphenyl)methyl]-2-methyl-  
(9CI) (CA INDEX NAME)

RN 302598-67-0 CAPLUS

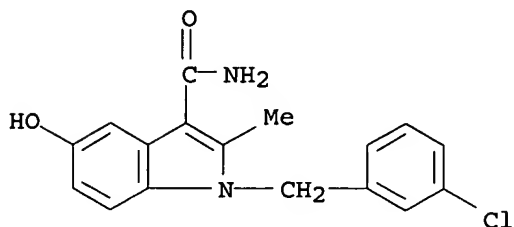
CN 1H-Indole-3-carboxamide, 5-hydroxy-2-methyl-1-[[4-(trifluoromethyl)phenyl]methyl]- (9CI) (CA INDEX NAME)



RN 302598-68-1 CAPLUS

CN 1H-Indole-3-carboxamide, 1-[(4-chlorophenyl)methyl]-5-hydroxy-2-methyl-  
(9CI) (CA INDEX NAME)

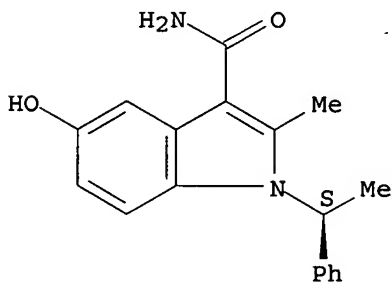
RN 302598-69-2 CAPLUS

CN 1H-Indole-3-carboxamide, 1-[(3-chlorophenyl)methyl]-5-hydroxy-2-methyl-  
(9CI) (CA INDEX NAME)

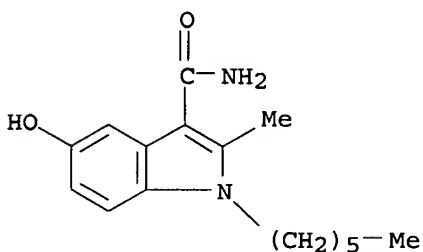
RN 302598-70-5 CAPLUS

CN 1H-Indole-3-carboxamide, 5-hydroxy-2-methyl-1-[(1S)-1-phenylethyl]- (9CI)  
(CA INDEX NAME)

Absolute stereochemistry.

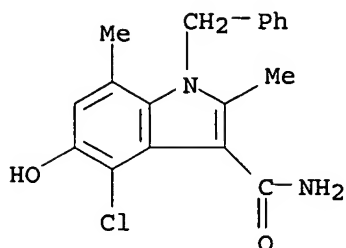


RN 302598-71-6 CAPLUS

CN 1H-Indole-3-carboxamide, 1-hexyl-5-hydroxy-2-methyl- (9CI) (CA INDEX  
NAME)

RN 354137-88-5 CAPLUS

CN 1H-Indole-3-carboxamide, 4-chloro-5-hydroxy-2,7-dimethyl-1-(phenylmethyl)-  
(9CI) (CA INDEX NAME)



L27 ANSWER 3 OF 11 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1998:274848 CAPLUS

DOCUMENT NUMBER: 129:45274

TITLE: Therapeutic uses and formulations of blood sugar-lowering indoles and their uses in preparation of pharmaceuticals

INVENTOR(S): Oku, Teruo; Sawada, Kozo; Kuroda, Akio; One, Kazuhiko; Yamazaki, Noritsugu; Imoto, Takafumi

PATENT ASSIGNEE(S): Fujisawa Pharmaceutical Co., Ltd., Japan

SOURCE: Jpn. Kokai Tokkyo Koho, 63 pp.

CODEN: JKXXAF

DOCUMENT TYPE: Patent

LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 10114654	A2	19980506	JP 1996-268402	19961009
PRIORITY APPLN. INFO.:			JP 1996-268402	19961009

OTHER SOURCE(S): MARPAT 129:45274

AB Pharmaceutical preps. containing indoles their pharmacol. acceptable salts are useful for prevention and/or treatment of glucose tolerance disorders, diabetes mellitus, hyperlipidemia, insulin resistance syndrome, cardiovascular disease, or hyperglycemia. The indoles are also useful in preparation of pharmaceuticals. Administration of

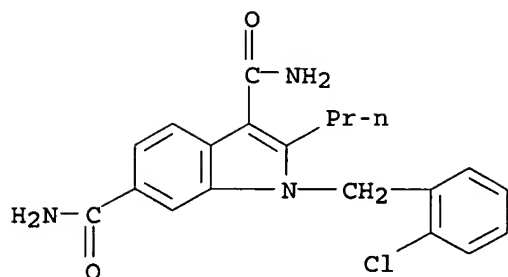
6-benzenesulfonylcarbamoyl-1-(2-chlorobenzyl)-2-methylindole at 300 mg/kg p.o. to db/db mice showed 70% lowering of blood sugar concns.

IT 184150-24-1P

RL: SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)  
(preparation and therapeutic uses of blood sugar-lowering indoles)

RN 184150-24-1 CAPLUS

CN 1H-Indole-3,6-dicarboxamide, 1-[(2-chlorophenyl)methyl]-2-propyl- (9CI)  
(CA INDEX NAME)



L27 ANSWER 4 OF 11 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1998:155177 CAPLUS

DOCUMENT NUMBER: 128:275074

TITLE: Cyclic nucleotide phosphodiesterase (PDE) inhibitors for prevention and treatment of lupus erythematosus and nephritis, and indoles as cGMP-PDE inhibitors

INVENTOR(S): Nomoto, Atsushi; Hamada, Kaori; Kodama, Hiroshi; Sokabe, Keizo

PATENT ASSIGNEE(S): Fujisawa Pharmaceutical Co., Ltd., Japan

SOURCE: Jpn. Kokai Tokkyo Koho, 61 pp.

CODEN: JKXXAF

DOCUMENT TYPE: Patent

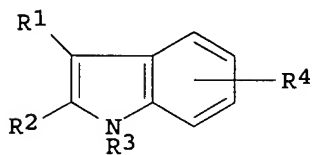
LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 10067682	A2	19980310	JP 1997-191618	19970716 <--
PRIORITY APPLN. INFO.: AU 1996-1188			19960723	
OTHER SOURCE(S): MARPAT 128:275074				

GI



I

AB Prophylactic and therapeutic agents for (systemic) lupus erythematosus and lupus nephritis contain cyclic nucleotide PDE inhibitors as active ingredients. Also claimed are indoles I [R1 = H, halo, NO2, (protected) CO2H, acyl, cyano, hydroxyimino-lower alkyl, (oxo-substituted) lower alkenyl, etc.; R2 = H, halo, lower alkenyl, acyl, (protected) CO2H, lower alkoxy, lower (hydroxy)alkyl; R3 = (un)substituted lower alkenyl, (un)substituted lower alkyl; R4 = (protected) CO2H, acyl, cyano, halo, heterocyclyl, (un)substituted NH2, (un)substituted alkyl; R1CCR2 may form (oxo-substituted) 4- to 7-membered heterocyclic ring] or their medically acceptable salts as cGMP-PDE inhibitors. 1-(6-Chloro-3,4-methylenedioxybenzyl)-3-methoxyacetyl-2-propylindole-6-carboxamide was effective in treatment of immune-complex nephritis in mice.

IT 184150-24-1P 205528-26-3P



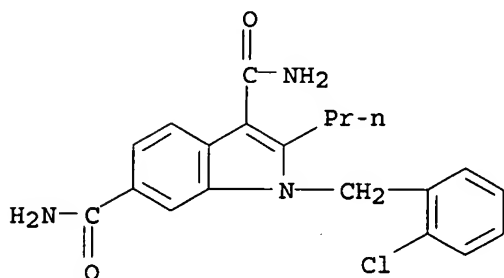
06/22/2004

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of indoles as cyclic nucleotide PDE inhibitors for treatment of lupus erythematosus and nephritis)

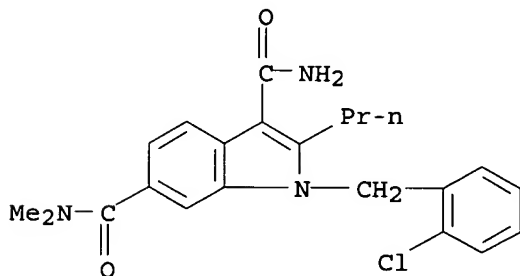
RN 184150-24-1 CAPLUS

CN 1H-Indole-3,6-dicarboxamide, 1-[(2-chlorophenyl)methyl]-2-propyl- (9CI)  
(CA INDEX NAME)



RN 205528-26-3 CAPLUS

CN 1H-Indole-3,6-dicarboxamide, 1-[(2-chlorophenyl)methyl]-N6,N6-dimethyl-2-propyl- (9CI) (CA INDEX NAME)



L27 ANSWER 5 OF 11 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1997:513631 CAPLUS

DOCUMENT NUMBER: 127:205572

TITLE: Preparation of thiazolylbenzofurans as leukotriene and SRS-A antagonists or inhibitors

INVENTOR(S): Matsuo, Masaaki; Okumura, Kazuo; Shigenaga, Shinji; Nishimura, Hiroaki; Matsuda, Hiroshi; Hagiwara, Daijiro; Terasaka, Tadashi

PATENT ASSIGNEE(S): Fujisawa Pharmaceutical Co., Ltd., Japan

SOURCE: PCT Int. Appl., 244 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

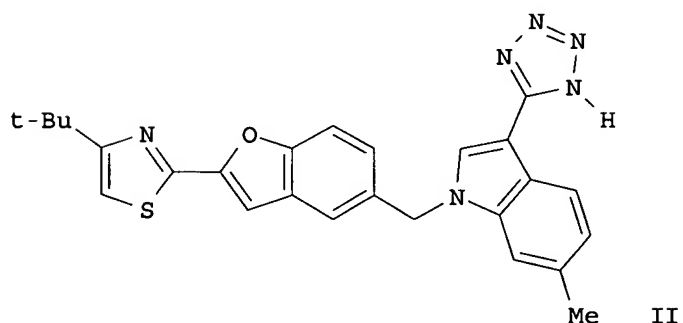
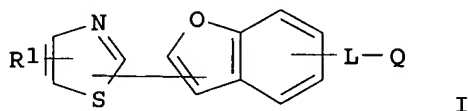
LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9727190	A1	19970731	WO 1997-JP73	19970117 <--
W: AU, CA, CN, HU, JP, KR, MX, SG, US, AM, AZ, BY, KG, KZ, MD, RU,				

TJ, TM  
 RW: AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE  
 ZA 9700415 A 19970730 ZA 1997-415 19970117 <--  
 CA 2244189 AA 19970731 CA 1997-2244189 19970117 <--  
 AU 9713991 A1 19970820 AU 1997-13991 19970117 <--  
 EP 880519 A1 19981202 EP 1997-900432 19970117 <--  
 EP 880519 B1 20020417  
 R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, PT, IE, FI  
 CN 1209809 A 19990303 CN 1997-191798 19970117 <--  
 JP 2000503984 T2 20000404 JP 1997-526720 19970117 <--  
 EP 1170009 A2 20020109 EP 2001-123263 19970117 <--  
 EP 1170009 A3 20020116  
 EP 1170009 B1 20040407  
 R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, PT, IE, FI  
 TW 474811 B 20020201 TW 1997-86100473 19970117 <--  
 AT 216384 E 20020515 AT 1997-900432 19970117 <--  
 ES 2171878 T3 20020916 ES 1997-900432 19970117 <--  
 AT 263561 E 20040415 AT 2001-123263 19970117  
 US 5994378 A 19991130 US 1998-101766 19980721 <--  
 PRIORITY APPLN. INFO.: GB 1996-1235 A 19960122  
 AU 1996-1111 A 19960718  
 AU 1996-9241 A 19960412  
 EP 1997-900432 A3 19970117  
 WO 1997-JP73 W 19970117  
 OTHER SOURCE(S): MARPAT 127:205572  
 GI

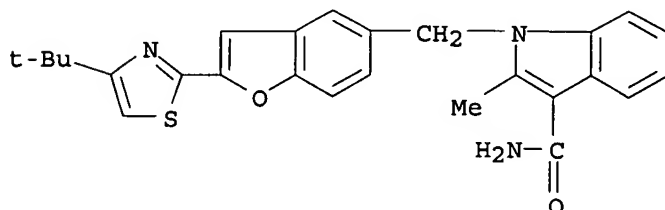


- AB The title compds. [I; R1 = lower alkyl; L = single bond, (un)substituted lower alkylene; Q = (un)substituted heterocyclic group, lower alkoxy substituted with aryl] which possess activities as leukotriene and SRS-A antagonists or inhibitors, and are useful in the treatment and/or prevention of allergy or inflammation, were prepared Thus, treatment of 4-tert-butyl-2-{5-[(3-cyano-6-methylindol-1-yl)methyl]benzofuran-2-yl}thiazole with NaN<sub>3</sub> and NH<sub>4</sub>Cl in DMF afforded the title compound II which showed IC<sub>50</sub> of < 5 nM against 3H-leukotriene D<sub>4</sub> receptor binding.
- IT 194488-60-3P 194488-61-4P  
 RL: BAC (Biological activity or effector, except adverse); BSU (Biological

study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use);  
 BIOL (Biological study); PREP (Preparation); USES (Uses)  
 (preparation of thiazolylbenzofurans as leukotriene and SRS-A antagonists or  
 inhibitors)

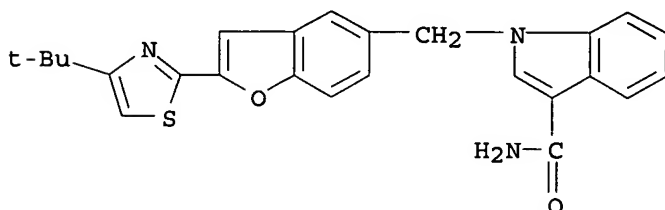
RN 194488-60-3 CAPLUS

CN 1H-Indole-3-carboxamide, 1-[[2-[4-(1,1-dimethylethyl)-2-thiazolyl]-5-  
 benzofuranyl]methyl]-2-methyl- (9CI) (CA INDEX NAME)



RN 194488-61-4 CAPLUS

CN 1H-Indole-3-carboxamide, 1-[[2-[4-(1,1-dimethylethyl)-2-thiazolyl]-5-  
 benzofuranyl]methyl]- (9CI) (CA INDEX NAME)



L27 ANSWER 6 OF 11 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1996:746234 CAPLUS

DOCUMENT NUMBER: 126:18786

TITLE: Indole derivatives as cGMP-PDE inhibitors

INVENTOR(S): Oku, Teruo; Sawada, Kozo; Kuroda, Akio; Ohne,  
 Kazuhiko; Nomoto, Atsushi; Hosogai, Naomi; Nakajima,  
 Yoshimitsu; Nagashima, Akira; Sogabe, Keizo; Amura,  
 Kouichi

PATENT ASSIGNEE(S): Fujisawa Pharmaceutical Co, Ltd., Japan

SOURCE: PCT Int. Appl., 211 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

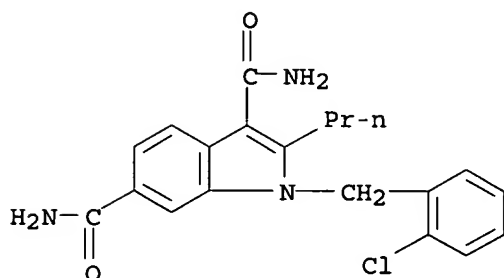
FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9632379	A1	19961017	WO 1996-JP892	19960402 <--
CA 2217707	AA	19961017	CA 1996-2217707	19960402 <--
AU 9651234	A1	19961030	AU 1996-51234	19960402 <--
AU 713460	B2	19991202		
EP 820441	A1	19980128	EP 1996-907750	19960402 <--
EP 820441	B1	20020626		

R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, PT, IE, FI

CN 1H-Indole-3,6-dicarboxamide, 1-[(2-chlorophenyl)methyl]-2-propyl- (9CI)  
(CA INDEX NAME)



L27 ANSWER 7 OF 11 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1995:982654 CAPLUS

DOCUMENT NUMBER: 124:175826

TITLE: Preparation of 2-indolyldisulfides and analogs as protein tyrosine kinase inhibitors and antitumor agents

INVENTOR(S): Dobrusin, Ellen M.; Showalter, Howard D. H.; Denny, William A.; Palmer, Brian D.; Rewcastle, Gordon W.; Tercel, Moana; Thompson, Andrew M.

PATENT ASSIGNEE(S): Warner-Lambert Co., USA

SOURCE: U.S., 53 pp. Cont.-in-part of U.S. Ser. No. 926, 015, abandoned.

CODEN: USXXAM

DOCUMENT TYPE: Patent

LANGUAGE: English

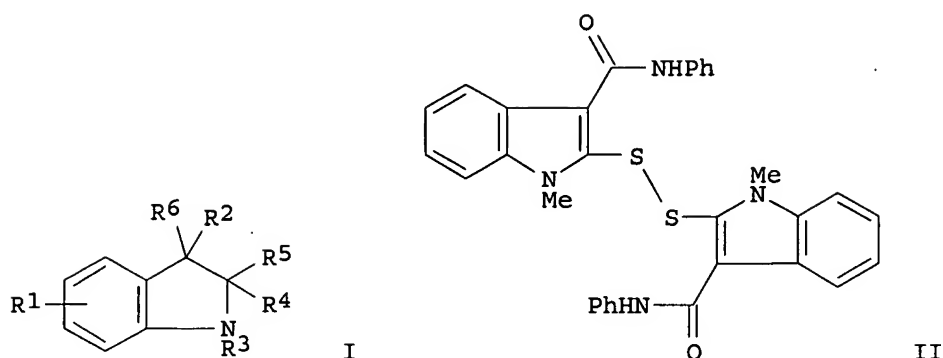
FAMILY ACC. NUM. COUNT: 2

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 5464861	A	19951107	US 1993-94792	19930809 <--
HU 71553	A2	19951228	HU 1995-341	19930802 <--
CZ 283965	B6	19980715	CZ 1995-288	19930802 <--
NZ 255194	A	20000128	NZ 1993-255194	19930802 <--
US 5556874	A	19960917	US 1995-438616	19950510 <--
PRIORITY APPLN. INFO.:			US 1992-926015	B2 19920806
			US 1993-94792	A3 19930809

OTHER SOURCE(S): MARPAT 124:175826

GI



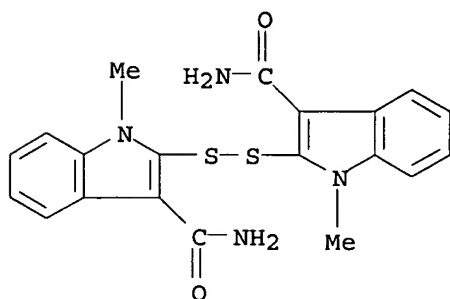
AB Title compds. [I; R1 = H, halo, alkyl, alkoxy, etc.; R2 = (acyl)alkyl, acyl, CH:CHCO<sub>2</sub>H, etc.; R3 = H, alkyl, CH<sub>2</sub>Ph; R4 = SH, SnR, SeH, SenR, etc.; R5 = H, alkyl, (hetero)aryl, I in which R4 = bond, etc.; R4R5 = S, Se; R5R6 = bond; R6 = H; n = 1-3] were prepared 2Hus, 1-methyl-2-indolinone was treated with P<sub>2</sub>S<sub>5</sub> and the product condensed with PhNCO to give, after oxidation, title compound II which had IC<sub>50</sub> of 3-4 μM against growth factor mediated mitogenesis in vitro.

IT 156136-31-1P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)  
(preparation of 2-indolyldisulfides and analogs as protein tyrosine kinase inhibitors and antitumor agents)

RN 156136-31-1 CAPLUS

CN 1H-Indole-3-carboxamide, 2,2'-dithiobis[1-methyl- (9CI) (CA INDEX NAME)



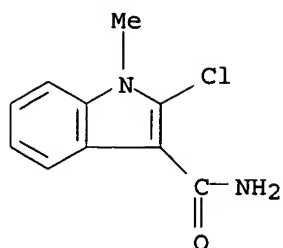
IT 120110-10-3, 2-Chloro-1-methylindole-3-carboxamide

RL: RCT (Reactant); RACT (Reactant or reagent)

(preparation of 2-indolyldisulfides and analogs as protein tyrosine kinase inhibitors and antitumor agents)

RN 120110-10-3 CAPLUS

CN 1H-Indole-3-carboxamide, 2-chloro-1-methyl- (9CI) (CA INDEX NAME)



L27 ANSWER 8 OF 11 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1994:483050 CAPLUS

DOCUMENT NUMBER: 121:83050

TITLE: Preparation of 2-indolinethiones and related disulfides and seleno-analogs as protein tyrosine kinase inhibitors and antitumor agents

INVENTOR(S): Dobrusin, Ellen Myra; Showalter, Howard Daniel Hollis; Denny, William Alexander; Palmer, Brian Desmond; Rewcastle, Gordon William; Tercel, Moana; Thompson, Andrew Mark

PATENT ASSIGNEE(S): Warner-Lambert Co., USA

SOURCE: PCT Int. Appl., 212 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

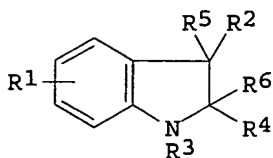
FAMILY ACC. NUM. COUNT: 2

PATENT INFORMATION:

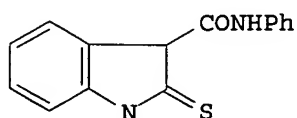
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9403427	A1	19940217	WO 1993-US7272	19930802 <--
W: AU, CA, CZ, FI, HU, JP, KR, NO, NZ, RU, SK				
RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
EP 654024	A1	19950524	EP 1993-918594	19930802 <--
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, MC, NL, PT, SE				
HU 71553	A2	19951228	HU 1995-341	19930802 <--
JP 08503450	T2	19960416	JP 1993-519671	19930802 <--
AU 672224	B2	19960926	AU 1993-47994	19930802 <--
AU 9347994	A1	19940303		
CZ 283965	B6	19980715	CZ 1995-288	19930802 <--
NZ 255194	A	20000128	NZ 1993-255194	19930802 <--
RU 2155187	C2	20000827	RU 1995-108332	19930802 <--
SK 283413	B6	20030701	SK 1995-135	19930802
PRIORITY APPLN. INFO.:			US 1992-926015	A 19920806
			WO 1993-US7272	W 19930802

OTHER SOURCE(S): MARPAT 121:83050

GI



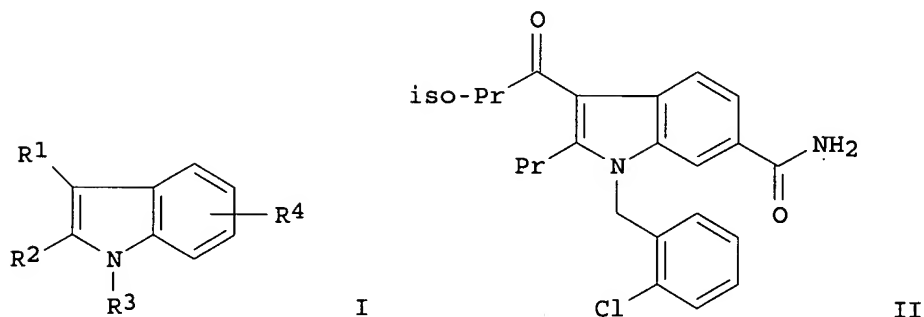
I



II

CN 1187812	A	19980715	CN 1996-194691	19960402	<--
JP 11503445	T2	19990326	JP 1996-530864	19960402	<--
AT 219765	E	20020715	AT 1996-907750	19960402	<--
ES 2175079	T3	20021116	ES 1996-907750	19960402	<--
ZA 9602859	A	19961011	ZA 1996-2859	19960410	<--
TW 420663	B	20010201	TW 1996-85104519	19960416	<--
US 6069156	A	20000530	US 1997-930597	19971210	<--
PRIORITY APPLN. INFO.:			GB 1995-7432	A	19950410
			GB 1995-12560	A	19950621
			GB 1995-16136	A	19950807
			AU 1996-8294	A	19960227
			WO 1996-JP892	W	19960402

OTHER SOURCE(S):            MARPAT 126:18786  
GI



AB The invention relates to new indole derivs. I and their pharmaceutically acceptable salts [wherein R<sup>1</sup> = H, halo, NO<sub>2</sub>, CO<sub>2</sub>H, protected CO<sub>2</sub>H, acyl, (un)substituted alk(en)yl, etc.; R<sup>2</sup> = H, halo, alkenyl, acyl, (un)substituted alkyl, etc.; R<sup>3</sup> = (un)substituted alk(en)yl where the substituent is oxo, (un)substituted aryl, or heterocyclyl; R<sup>4</sup> = CO<sub>2</sub>H, protected CO<sub>2</sub>H, acyl, cyano, amino, halo, etc.; R<sup>1</sup> and R<sup>2</sup> may form 4- to 7-membered carboxylic ring (un)substituted with oxo]. I are cyclic nucleotide-PDE inhibitors (specifically cGMP-PDE), and are useful for treating and preventing a variety of conditions, including angina, hypertension, renal failure, atherosclerosis, stroke, asthma, impotence, diabetic complications, and glaucoma. Almost 300 compds. I and numerous intermediates were prepared. For example, Me 3-isobutyryl-2-propylindole-6-carboxylate (preparation given) was N-benzylated by 2-chlorobenzyl bromide using NaH in DMF. The product underwent saponification with NaOH in aqueous

EtOH, followed by amidation of the resultant acid using EDC, HOBT, and aqueous NH<sub>3</sub>, to give title amide II. II inhibited human platelet cGMP-PDE in vitro with IC<sub>50</sub> <100 nM. I were also active in a variety of other bioassays, including relaxation of isolated rat aorta, inhibition of vascular smooth muscle cell proliferation, inhibition of vasopressin-induced vasospasm, the cyclosporin and FK506 nephritis models, the diabetic glomerulosclerosis model, and several animal impotence models.

IT 184150-24-1P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)  
(preparation of indole derivs. as cGMP-PDE inhibitors)

RN 184150-24-1 CAPLUS

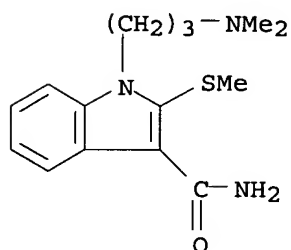
AB Title compds. [I; R1 = H, halo, OH, alkyl, alkoxy, CO<sub>2</sub>H, etc.; 1 or 2 CR1 = N; R2 = (acyl)alkyl, CH:CHCO<sub>2</sub>H, alkylcarbonyl, acyl, etc.; R3 = H, alkyl, CH<sub>2</sub>Ph; R4 = ZH, ZnX, ZnQ; R5 = H and R4R6 = S or Se; R5R6 = bond; Q = I in which R4 = Zn and R5R6 = bond; X = H, alkyl, CH<sub>2</sub>Ph, (hetero)aryl; Z = S, Se; n = 0-3] were prepared Thus, 1-methyl-2-indolinone was treated with P<sub>2</sub>S<sub>5</sub> and the product treated with NaH and PhNCO to give indolinethionecarboxamide II which had IC<sub>50</sub> of 2μM against epidermal growth factor mediated mitogenesis.

IT 156137-01-8P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
(preparation and reaction of, in preparation of protein tyrosine kinase inhibitor)

RN 156137-01-8 CAPLUS

CN 1H-Indole-3-carboxamide, 1-[3-(dimethylamino)propyl]-2-(methylthio)- (9CI)  
(CA INDEX NAME)

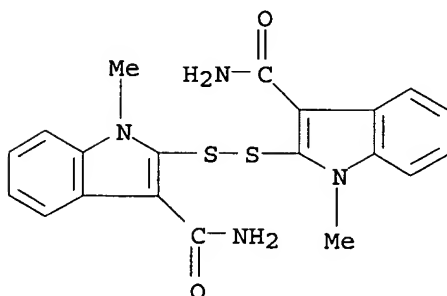


IT 156136-31-1P

RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation of, as protein tyrosine kinase inhibitor)

RN 156136-31-1 CAPLUS

CN 1H-Indole-3-carboxamide, 2,2'-dithiobis[1-methyl- (9CI) (CA INDEX NAME)



IT 120110-10-3

RL: RCT (Reactant); RACT (Reactant or reagent)  
(reaction of, in preparation of protein tyrosine kinase inhibitor)

RN 120110-10-3 CAPLUS

CN 1H-Indole-3-carboxamide, 2-chloro-1-methyl- (9CI) (CA INDEX NAME)



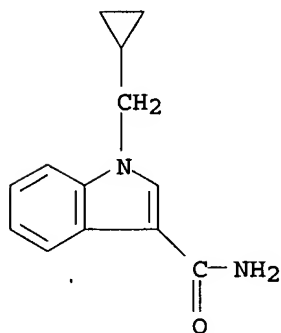
IT 128200-23-7P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and reaction of, in preparation of serotonergic S3 antagonists)

RN 128200-23-7 CAPLUS

CN 1H-Indole-3-carboxamide, 1-(cyclopropylmethyl)- (9CI) (CA INDEX NAME)



L27 ANSWER 10 OF 11 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1990:139035 CAPLUS

DOCUMENT NUMBER: 112:139035

TITLE: Five-membered heterocycles as pharmaceuticals

INVENTOR(S): Baker, Raymond; Saunders, John; Swain, Christopher

PATENT ASSIGNEE(S): Merck Sharp and Dohme Ltd., UK

SOURCE: Eur. Pat. Appl., 39 pp.

CODEN: EPXXDW

DOCUMENT TYPE:

Patent

LANGUAGE:

English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

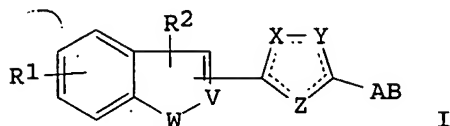
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 328200	A1	19890816	EP 1989-200244	19890203 <--
EP 328200	B1	19931208		
R: AT, BE, CH, DE, ES, FR, GB, GR, IT, LI, LU, NL, SE				
US 4952587	A	19900828	US 1989-306007	19890203 <--
AT 98241	E	19931215	AT 1989-200244	19890203 <--
ES 2061928	T3	19941216	ES 1989-200244	19890203 <--
ZA 8900921	A	19900228	ZA 1989-921	19890207 <--
JP 01268687	A2	19891026	JP 1989-28813	19890209 <--
JP 2505875	B2	19960612		
FI 8900657	A	19890813	FI 1989-657	19890210 <--
DK 8900616	A	19890813	DK 1989-616	19890210 <--
NO 8900594	A	19890814	NO 1989-594	19890210 <--
AU 8929860	A1	19890817	AU 1989-29860	19890210 <--
AU 614027	B2	19910815		
CA 1337199	A1	19951003	CA 1989-590772	19890210 <--
US 5041456	A	19910820	US 1990-552395	19900713 <--

PRIORITY APPLN. INFO.:

GB 1988-3317	19880212
GB 1988-10789	19880506
EP 1989-200244	19890203
US 1989-306007	19890203

GI

10714568



AB Title compds. I [X, Y, Z = O, S, N, C and at least one of X, Y, and Z = O, S, N; the dotted circle = one or two double bonds in any position; R1 = H, OH, alkyl, alkenyl, alkynyl, amino, cyano, etc.; R2 = H, halo, alkyl, alkoxy, alkylcarbonyl; V = CH, C (when bond with the 5-membered ring); W = O, S, NR3 (R3 = H, alkyl, alkenyl, alkynyl); A = bond, (substituted) alkylene; B = non-aromatic aza(bi)cyclyl, NR4R5 (R4, R5 = H, alkyl, alkenyl, alkynyl, aralkyl)] are prepared I are useful for treating psychotic disorders (e.g. schizophrenia, mania), anxiety, alc. or drug withdrawal, pain, gastric stasis, gastric dysfunction (e.g. peptic ulcer, esophageal reflux, flatulence), migraine, nausea, vomiting, and presenile and senile dementia (Alzheimer's disease) (no data). A mixture of H2NOH, HCl, ~~K2CO3~~, and 1-methylindole-3-nitrile in EtOH was refluxed to give 1-methylindol-3-ylamide oxime, which in DMF in the presence of mol. sieves was successively treated with NaH and 3-carbomethoxy-1-azabicyclo[2.2.2]octane to give 3-[3-(methylindol-3-yl)-1,2,4-oxadiazol-5-yl]-1-azabicyclo[2.2.2]octane.

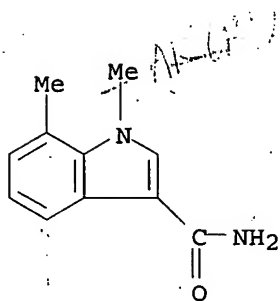
IT 125818-12-4P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and reaction of, in preparation of pharmaceuticals)

RN 125818-12-4 CAPLUS

CN 1H-Indole-3-carboxamide, 1,7-dimethyl- (9CI) (CA INDEX NAME)



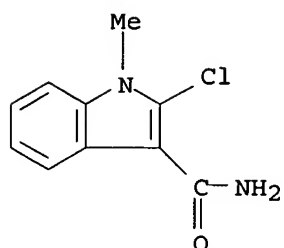
IT 118959-44-7

RL: RCT (Reactant); RACT (Reactant or reagent)

(reaction of, in preparation of pharmaceuticals)

RN 118959-44-7 CAPLUS

CN 1H-Indole-3-carboxamide, 1-methyl- (9CI) (CA INDEX NAME)



L27 ANSWER 9 OF 11 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1990:552390 CAPLUS

DOCUMENT NUMBER: 113:152390

TITLE: Preparation of spirocyclic compounds incorporating five-membered rings with two heteroatoms, especially spiro[azabicyclooctaneoxazoles], useful as drugs

INVENTOR(S): Baker, Raymond; Kneen, Clare O.; Saunders, John; Swain, Christopher

PATENT ASSIGNEE(S): Merck Sharp and Dohme Ltd., UK

SOURCE: Eur. Pat. Appl., 38 pp.

CODEN: EPXXDW

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

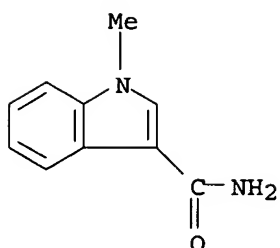
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 337547	A1	19891018	EP 1989-200862	19890406 <--
EP 337547	B1	19940302		
R: AT, BE, CH, DE, ES, FR, GB, GR, IT, LI, LU, NL, SE				
FI 8901584	A	19891012	FI 1989-1584	19890403 <--
US 4940703	A	19900710	US 1989-333076	19890404 <--
AT 102205	E	19940315	AT 1989-200862	19890406 <--
ES 2061933	T3	19941216	ES 1989-200862	19890406 <--
AU 8932632	A1	19891012	AU 1989-32632	19890410 <--
AU 617785	B2	19911205		
DK 8901704	A	19891012	DK 1989-1704	19890410 <--
NO 8901471	A	19891012	NO 1989-1471	19890410 <--
JP 01305092	A2	19891208	JP 1989-88177	19890410 <--
ZA 8902587	A	19900328	ZA 1989-2587	19890410 <--
PRIORITY APPLN. INFO.:			GB 1988-8433	19880411
			EP 1989-200862	19890406

OTHER SOURCE(S): MARPAT 113:152390

GI For diagram(s), see printed CA Issue.

AB Title compds. I [R1 = H, OH, alkyl, alkenyl, alkynyl, alkoxy, PhCH2O, hydroxyalkyl, halo, amino, cyano, NO2, (substituted) carbamoyl or sulfamoyl; R2 = H, halo, alkyl, alkoxy, alkylcarbonyl; V = N, CH, C; W = O, S, (substituted) NH; 2 of X, Y, Z = O, S, N; other = C; or Y = CO; Q = residue of aza(bi)cyclic system], some of which act on 5-HT3 receptors (no data), are prepared for treatment of psychosis, anxiety, gastric dysfunction, nausea, senile dementia, etc. Thus, treatment of 1-methyl-1H-indole-3-nitrile with dry HCl in MeOH gave the Me imidate HCl salt, which underwent cyclocondensation with 3-aminomethyl-3-hydroxy-1-azabicyclo[2.2.2]octane di-HCl in refluxing MeOH to give, after acidification, (methylindolyl)spiro[azabicyclooctaneoxazole] II as the di-HCl salt.



L27 ANSWER 11 OF 11 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1989:23730 CAPLUS

DOCUMENT NUMBER: 110:23730

TITLE: 5-Hydroxyindole-3-carboxamide derivatives as diuretics and cardiovascular agents, their preparation, and formulations containing them

INVENTOR(S): Tahara, Tetsuya; Ikabe, Tsuguo; Hakamada, Ichiro; Yaoka, Osamu

PATENT ASSIGNEE(S): Yoshitomi Pharmaceutical Industries, Ltd., Japan

SOURCE: PCT Int. Appl., 30 pp.

CODEN: PIXXD2

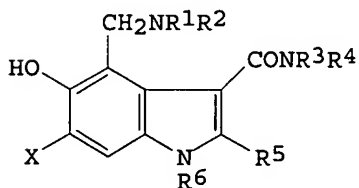
DOCUMENT TYPE: Patent

LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 8805432	A1	19880728	WO 1988-JP35	19880119 <--
W: US				
RW: AT, BE, CH, DE, FR, GB, IT, NL, SE				
EP 299076	A1	19890118	EP 1988-900852	19880119 <--
R: AT, BE, CH, DE, FR, GB, IT, LI, NL, SE				
JP 63301862	A2	19881208	JP 1988-11225	19880121 <--
US 4874759	A	19891017	US 1988-261836	19880923 <--
PRIORITY APPLN. INFO.:			JP 1987-14943	19870123
			WO 1988-JP35	19880119
OTHER SOURCE(S):			CASREACT 110:23730; MARPAT 110:23730	
GI				



I

AB The title compds. I (R1-R4 = H, alkyl, aryl, aralkyl, heteroaryl, or NR1R2, NR3R4 = heterocyclyl; R5 = alkyl; R6 = H, alkyl, cycloalkyl, etc.; X = H, halo, lower alkanoyl) and acid addition salts thereof, useful as diuretics and agents for the treatment of circulation disorders, were prepared Reaction of N,N-dibutyl-5-hydroxy-2-methyl-1-(2-phenylethyl)indole-3-carboxamide with piperidine and HCHO, followed by Friedel-Crafts

reaction with  $\text{MeCH}_2\text{COCl}$ , gave N,N-dibutyl-5-hydroxy-2-methyl-1-(2-phenylethyl)-4-piperidinomethyl-6-propionylindole-3-carboxamide (II). II increased coronary blood flow with an  $\text{ED}_{50}$  of  $12 \mu\text{g}$  i.v. in dogs. Tablets containing 4-(6-bromo-5-hydroxy-2-methyl-4-piperidinomethyl-1H-indol-3-ylcarbonyl)morpholine 5, starch 15, lactose 60, microcryst. cellulose 16, talc 3, and Mg stearate 1 mg were prepared

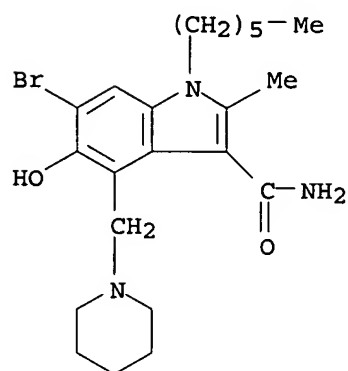
IT 118052-76-9P 118052-94-1P

RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation of, as diuretic and agent for treatment of circulation disorders)

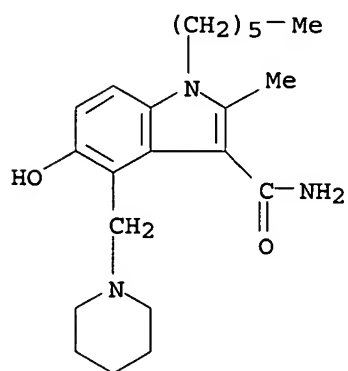
RN 118052-76-9 CAPLUS

CN 1H-Indole-3-carboxamide, 6-bromo-1-hexyl-5-hydroxy-2-methyl-4-(1-piperidinylmethyl)- (9CI) (CA INDEX NAME)



RN 118052-94-1 CAPLUS

CN 1H-Indole-3-carboxamide, 1-hexyl-5-hydroxy-2-methyl-4-(1-piperidinylmethyl)- (9CI) (CA INDEX NAME)



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COST IN U.S. DOLLARS

SINCE FILE	TOTAL
ENTRY	SESSION
89.81	1080.23

FULL ESTIMATED COST

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE	TOTAL
ENTRY	SESSION
-11.78	-18.02

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